Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

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Overview of Invited Talks and Sessions

(Lecture rooms: H 0104, H 0110, H 2053, H 3005, H 3010, and A 053; Posters: B)

Invited and Topical Talks except for Focus Sessions

TT 4.1	Mon	9:30–10:00	H 0104	**Entanglement in the Many-Body Localized Phase and Transition** — •Jens H. Bardarson
TT 20.1	Mon	15:00–15:30	A 053	**The Wires' Approach to Topological Insulators** — •Yuval Oreg
TT 31.1	Tue	9:30–10:00	H 2053	**Electronic Correlations in Hole- and Electron-Doped Fe-Based Superconductors and Evidence for the C_4-Magnetic Phase in $Ba_{1-x}K_xFe_2As_2$** — •Frédéric Hardy
TT 32.7	Tue	11:15–11:45	H 3005	**Interacting Topological Insulators** — •Stephan Rachel
TT 43.1	Tue	14:00–14:30	H 2053	**Magnetism and Superconductivity in Eu-Based Iron Pnictides** — •Sina Zapf
TT 65.1	Wed	15:00–15:30	H 0104	**Strong Correlations in Disordered One-Dimensional Systems** — •Christoph Karrasch
TT 68.7	Wed	16:45–17:15	H 3010	**Structural Stability and Lattice Dynamics of Correlated Electron Materials** — •Ivan Leonov
TT 66.9	Wed	17:15–17:45	H 2053	**Probing Andreev Bound States in One-Atom Superconducting Contacts** — •Hugues Pothier
TT 85.1	Thu	9:30–10:00	H 2053	**A Brisk Walk through Phase Transitions in Time: Oscillating Order and the Dynamics of Topological Defects** — •Dragan Mihailovic
TT 102.7	Thu	16:45–17:15	A 053	**Microscopic Origin of the 0.7-Anomaly in Quantum Point Contacts: Correlations in 1D** — •Stefan Ludwig

Tutorial "Nonequilibrium Renormalization Group Methods"

TT 1.1	Sun	16:05–16:45	H 0110	**From Lunar Motion to Real Time Evolution of Quantum Many-Body Systems** — •Stefan Kehrein
TT 1.2	Sun	16:50–17:30	H 0110	**Functional Renormalization Group Approach to Nonequilibrium Transport through Mesoscopic Systems** — •Severin Georg Jakobs
TT 1.3	Sun	17:35–18:15	H 0110	**Real-Time RG: Nonequilibrium Properties of Open Quantum Systems** — •Herbert Schoeller

Tutorial "Ferroics" (organized by DF)

DF 1.1	Sun	16:00–16:50	H 0107	**Fundamentals of ferroelectric materials** — •Susan Trolier-McKinstry
DF 1.2	Sun	16:50–17:40	H 0107	**Domain walls in multiferroics as functional oxide interfaces** — •Manfred Fiebig
DF 1.3	Sun	17:40–18:30	H 0107	**Ferroelastic templates for multiferroic domain boundaries** — •Ekhard Salje

Tutorial "Density Functional Theory: A Computational Path to Interesting Spin-Textures and Novel Skyrmions" (organized by MA)

MA 1.1	Sun	16:05–16:50	H 1012	**Introduction to Spin-Density-Functional Theory** — •Nicole Helbig
MA 1.2	Sun	16:50–17:35	H 1012	**Determining chiral magnetism from density functional theory** — •Stefan Blügel
MA 1.3	Sun	17:45–18:30	H 1012	**Magneto-transport properties in spiralling spin textures** — •Yuriy Mokrousov

Invited and Topical Talks of the Focus Session "Skyrmionics: Future of Spintronics?"

TT 15.1	Mon	15:00–15:30	H 0104	**Skyrmion Dynamics** — •Yoshinori Tokura
TT 15.2	Mon	15:30–16:00	H 0104	**Topological Transport Phenomena in Magnetic Skyrmion Matter** — •Markus Garst
TT 15.3	Mon	16:00–16:30	H 0104	**Interface Induced Individual Skyrmions in Thin Films and Multilayers** — •A. Fert
TT 15.4	Mon	16:45–17:15	H 0104	**Magnetic Skyrmions and Chiral Spin Structures in Ultra-Thin Films** — •Stefan Blügel
TT 15.5	Mon	17:15–17:45	H 0104	**Racetrack Memory: Highly Efficient Current Induced Domain Wall Motion in Synthetic Antiferromagnetic Racetracks** — •Stuart Parkin

Invited and Topical Talks of the Focus Session "Dynamics in Many-Body Systems: Equilibration and Localization"

TT 29.1	Tue	9:30–10:00	H 0104	**Probing Non-Equilibrium Dynamics with Ultracold Atoms: from Quantum Magnetism to Many-Body Localization** — •Immanuel Bloch
TT 29.2	Tue	10:00–10:30	H 0104	**Many-Body Localization** — •Dmitry Abanin
TT 29.3	Tue	10:30–11:00	H 0104	**Long-Time Behaviour of Periodically Driven Many-Body Quantum Systems** — •Achilleas Lazarides
TT 29.4	Tue	11:15–11:45	H 0104	**Many Body Localization and Eigenstate Order** — •Shivaji Sondhi
TT 29.5	Tue	11:45–12:15	H 0104	**Anderson Transitions and Electron-Electron Interaction** — •Alexander Mirlin

Invited and Topical Talks of the Focus Session "Electric Power Applications of Superconductivity"

TT 51.1	Wed	9:30–10:00	H 0104	**High Power Equipment based on High-Temperature Superconductors: the Added Value from an Industrial Point of View** — •Tabea Arndt
TT 51.2	Wed	10:00–10:30	H 0104	**Conductors and Cables from REBCO High Temperature Superconductors for Applications** — •Wilfried Goldacker
TT 51.3	Wed	10:30–11:00	H 0104	**Power Transmission via Superconducting Lines** — •Amalia Ballarino
TT 51.4	Wed	11:15–11:45	H 0104	**High field transport properties of MBE processed Fe-based superconducting thin films** — •Kazumasa Iida
TT 51.5	Wed	11:45–12:15	H 0104	**Advanced Superconducting Power Cable for MV Urban Power Supply** — •Frank Schmidt

Invited and Topical Talks of the Focus Session "Nanoscopic Superconducting Heterostructures"

TT 84.1	Thu	9:30–10:00	H 0104	**Creating and Manipulating Nonequilibrium Spins in Nanoscale Superconductors** — •Detlef Beckmann
TT 84.2	Thu	10:00–10:30	H 0104	**Non-Equilibrium Effects in a Josephson Junction Coupled to a Precessing Spin** — •Mikael Fogelström
TT 84.3	Thu	10:30–11:00	H 0104	**Signature of Magnetic-Dependent Gapless Odd Frequency States at Superconductor / Ferromagnet Interfaces** — •Jason Robinson
TT 84.4	Thu	11:15–11:45	H 0104	**Thermoelectric Effects and Spin Injection into Superconductors with Exchange Field** — •Tero Heikkilä
TT 84.5	Thu	11:45–12:15	H 0104	**Spin Injection and Relaxation in a Mesoscopic Superconductor** — •Marco Aprili

Invited and Topical Talks of the Focus Session "Visualization of Heavy Fermion Formation through Scanning Tunneling Microscopy"

TT 98.1	Thu	15:00–15:30	H 0104	**Scanning Tunneling Spectroscopy: a New Tool for Probing Heavy Fermion Materials** — •Piers Coleman
TT 98.2	Thu	15:30–16:00	H 0104	**The Single-Atom Kondo Effect as a Local Probe for Magnetic Interactions** — •Jörg Kröger
TT 98.3	Thu	16:00–16:30	H 0104	**Correlated Electrons under the Microscope: from Atomic Scale Model Systems to Bulk Materials** — •Peter Wahl
TT 98.4	Thu	16:45–17:15	H 0104	**Developing Kondo Lattice Coherence and Quantum Criticality in $YbRh_2Si_2$** — •Steffen Wirth
TT 98.5	Thu	17:15–17:45	H 0104	**Visualizing the Formation and Magnetically-Mediated Cooper Pairing of Heavy Fermions** — •JC Seamus Davis

Invited Talks of the Joint Symposium SYDW "Domain Wall Functionality and Engineering in Complex Oxides"

See SYDW for the full program of the symposium.

SYDW 1.1	Mon	9:30–10:00	H 0105	**Domain walls: from conductive paths to technology roadmaps** — •Gustau Catalan
SYDW 1.2	Mon	10:00–10:30	H 0105	**Domain walls and oxygen vacancies - towards reversible control of domain wall conductance** — •Patrycja Paruch
SYDW 1.3	Mon	10:30–11:00	H 0105	**Novel mechanisms of domain-wall formation** — •Andres Cano
SYDW 1.4	Mon	11:30–12:00	H 0105	**Novel materials at domain walls** — •Beatriz Noheda
SYDW 1.5	Mon	12:00–12:30	H 0105	**Controlling and mapping domain wall behaviour in ferroelectrics** — •John Martin Gregg

Invited Talks of the Joint Symposium SYHM "Higgs Modes in Condensed Matter and Quantum Gases"

See SYHM for the full program of the symposium.

SYHM 1.1	Wed	15:00–15:30	H 0105	**Amplitude or Higgs Modes in Condensed Matter** — •Chandra Varma
SYHM 1.2	Wed	15:30–16:00	H 0105	**Higgs Particles for Systems with U(1) Symmetry in Two Dimensions** — •Lode Pollet
SYHM 1.3	Wed	16:00–16:30	H 0105	**Massive Photons and the Anderson-Higgs Mechanism in Superconductors** — •Dirk van der Marel
SYHM 1.4	Wed	16:45–17:15	H 0105	**Amplitude Higgs Mode in $2H$-$NbSe_2$ Superconductor** — •Marie-Aude Méasson
SYHM 1.5	Wed	17:15–17:45	H 0105	**The Higgs Mode in Disordered Superconductors Close to a Quantum Phase Transition** — •Aviad Frydman

Invited Talks of the Joint Symposium SYMM "Magic MAX Phases: Self-healing, Magnetism and the Next Best Graphene"

See SYMM for the full program of the symposium.

SYMM 1.1	Thu	9:30–10:15	H 0105	**From MAX to MXene - From 3D to 2D** — •Michel Barsoum
SYMM 1.2	Thu	10:15–10:45	H 0105	**Structure evolution during low temperature growth of nanolaminate thin films** — •J.M. Schneider
SYMM 1.3	Thu	11:00–11:30	H 0105	**Autonomous healing of crack damage in MAX phase ceramics** — •Willem G. Sloof
SYMM 1.4	Thu	11:30–12:00	H 0105	**Magnetic MAX phases from first principles and thin film synthesis** — •Johanna Rosen
SYMM 1.5	Thu	12:00–12:30	H 0105	**Weak Field Magneto-Transport Properties of Mn+1AXn Phases** — •Thierry Ouisse

Invited Talks of the Joint Symposium SYGP "Geometric Paradigms in Modern Physics"

See SYGP for the full program of the symposium.

SYGP 1.1	Thu	15:00–15:30	H 0105	**General relativity: a theory born in creative confusion** — •Harvey Brown
SYGP 1.2	Thu	15:30–16:00	H 0105	**Gravitating Non-Abelian Fields: Solitons and Black Holes** — •Jutta Kunz
SYGP 1.3	Thu	16:00–16:30	H 0105	**Geometric principles in the physics of topological matter** — •Alexander Altland
SYGP 1.4	Thu	16:30–17:00	H 0105	**General Covariance in Quantum Field Theory on Curved Spacetimes** — •Thomas-Paul Hack
SYGP 1.5	Thu	17:00–17:30	H 0105	**The (noncommutative) Geometry of the Standard Model of Particle Physics** — •Christoph Stephan

Invited Talks of the Joint Symposium SYME "Frontiers of Electronic Structure Theory: Many-body Effects on the Nano-Scale"

See SYME for the full program of the symposium.

SYME 1.1	Fri	9:30–10:00	H 0105	**Excitations and charge transfer phenomena in C based systems** — •Elisa Molinari
SYME 1.2	Fri	10:00–10:30	H 0105	**Towards optimal correlation factors for many-electron perturbation theories** — •Andreas Grüneis
SYME 1.3	Fri	10:30–11:00	H 0105	**Towards an ab-initio description of high temperature superconductivity** — •Garnet Chan
SYME 1.4	Fri	11:15–11:45	H 0105	**Correlation effects in unconventional superconductors: from micro- to nano- and macroscales.** — •Roser Valenti
SYME 1.5	Fri	11:45–12:15	H 0105	**Stochastic density functional and GW theories scaling linearly with system size** — •Roi Baer

Sessions

TT 1.1–1.3	Sun	16:00–18:15	H 0110	**Tutorial: Nonequilibrium Renormalization Group Methods**
TT 2.1–2.3	Sun	16:00–18:30	H 0107	**Tutorial: Ferroics (organized by DF)**
TT 3.1–3.3	Sun	16:00–18:30	H 1012	**Tutorial: Density Functional Theory: A Computational Path to Interesting Spin-Textures and Novel Skyrmions (organized by MA)**
TT 4.1–4.12	Mon	9:30–13:00	H 0104	**Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 1 (jointly with DY)**
TT 5.1–5.13	Mon	9:30–13:00	H 0110	**Correlated Electrons: Spin Systems and Itinerant Magnets – Frustrated Magnets 1 (jointly with MA)**
TT 6.1–6.11	Mon	9:30–12:30	H 2053	**Superconductivity: Cryodetectors**
TT 7.1–7.13	Mon	9:30–13:00	H 3005	**Transport: Quantum Coherence and Quantum Information Systems – Theory (jointly with HL, MA)**
TT 8.1–8.11	Mon	9:30–12:30	H 3010	**Low-Dimensional Systems: Oxide Hetero-Interfaces**
TT 9.1–9.9	Mon	9:30–12:00	A 053	**Transport: Spintronics and Magnetotransport (jointly with HL, MA)**
TT 10.1–10.14	Mon	9:30–13:00	H 2032	**Organic Electronics and Photovoltaics (organized by DS)**
TT 11.1–11.12	Mon	9:30–12:45	H 0112	**Magnetic Heuslers, Half-Metals and Oxides (jointly with MA)**
TT 12.1–12.8	Mon	9:30–11:30	ER 270	**Graphene: THz, NIR, and Transport Properties (jointly with HL, O)**
TT 13.1–13.12	Mon	9:30–13:15	EW 201	**Focus Session: Functional Semiconductor Nanowires I (organized by HL)**
TT 14.1–14.12	Mon	9:30–12:45	EB 301	**Surface Magnetism – Skyrmions (jointly with MA, O)**
TT 15.1–15.5	Mon	15:00–17:45	H 0104	**Focus Session: Skyrmionics: Future of Spintronics? (jointly with MA)**
TT 16.1–16.9	Mon	15:00–17:15	H 0110	**Transport: Quantum Coherence and Quantum Information Systems – Experiments (jointly with HL, MA)**

TT 17.1–17.14	Mon	15:00–18:45	H 2053	**Superconductivity: Properties and Electronic Structure**
TT 18.1–18.13	Mon	15:00–18:30	H 3005	**Correlated Electrons: Spin Systems and Itinerant Magnets – Frustrated Magnets 2 (jointly with MA)**
TT 19.1–19.11	Mon	15:00–18:00	H 3010	**Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 2 (jointly with DY)**
TT 20.1–20.9	Mon	15:00–17:45	A 053	**Transport: Topological Insulators 1 (jointly with DS, HL, MA, O)**
TT 21.1–21.54	Mon	15:00–18:00	Poster B	**Superconductivity: Poster Session**
TT 22.1–22.4	Mon	15:00–18:00	Poster B	**Other Low Temperature Topics: Poster Session**
TT 23.1–23.14	Mon	15:00–18:45	H 1012	**Magnetic Heuslers, Half-Metals, Semiconductors, and Oxides (organized by MA)**
TT 24.1–24.12	Mon	15:00–18:45	EW 201	**Focus Session: Functional Semiconductor Nanowires II (organized by HL)**
TT 25.1–25.13	Mon	15:00–18:45	BH-N 243	**Brownian Motion and Transport (jointly with DY, CPP)**
TT 26.1–26.13	Mon	15:00–18:30	BH-N 334	**Quantum Dynamics, Decoherence and Quantum Information (jointly with DY)**
TT 27.1–27.9	Mon	15:00–17:15	ER 164	**Graphene: Theory (jointly with HL, O)**
TT 28.1–28.30	Mon	19:00–21:00	Poster C	**Poster Session on Ferroic Domain Walls - Multiferroics (jointly with DF, KR, MA)**
TT 29.1–29.8	Tue	9:30–13:00	H 0104	**Focus Session: Dynamics in Many-Body Systems: Equilibration and Localization (joint session TT/DY)**
TT 30.1–30.13	Tue	9:30–13:00	H 0110	**Correlated Electrons: Spin Systems and Itinerant Magnets – Frustrated Magnets 3 (jointly with MA)**
TT 31.1–31.11	Tue	9:30–12:45	H 2053	**Superconductivity: Fe-based Superconductors – 122 and 111**
TT 32.1–32.12	Tue	9:30–13:00	H 3005	**Transport: Topological Insulators 2 (jointly with DS, HL, MA, O)**
TT 33.1–33.10	Tue	9:30–12:15	H 3010	**Low-Dimensional Systems: Other Materials**
TT 34.1–34.10	Tue	9:30–12:15	A 053	**Transport: Graphene (jointly with CPP, DS, DY, HL, MA, O)**
TT 35.1–35.16	Tue	9:30–16:30	EB 301	**PhD Symposium: Quantum Phase Transitions: Emergent Phenomena beyond Elementary Excitations (organized by MA, jDPG)**
TT 36.1–36.13	Tue	9:30–13:00	C 130	**Organic Electronics and Photovoltaics: Transport of Charges – from Molecules to Devices (jointly with CPP, HL)**
TT 37.1–37.6	Tue	9:30–11:00	H 0111	**Thermoelectric Materials (organized by DS)**
TT 38.1–38.11	Tue	10:30–13:30	MA 004	**Frontiers of Electronic Structure Theory: Nuclear Dynamics, Methods (jointly with O, HL)**
TT 39.1–39.10	Tue	10:30–13:00	MA 041	**Graphene: Growth & Intercalation (jointly with O, HL)**
TT 40.1–40.11	Tue	9:30–12:30	H 0112	**Electronic Structure of Magnetism, Micromagnetism, Computational Magnetism (organized by MA)**
TT 41.1–41.8	Tue	9:30–11:30	ER 270	**Spintronics: Excitons and Local Spins (jointly with HL, MA)**
TT 42.1–42.8	Tue	14:00–16:00	H 0110	**Transport: Topological Insulators 3 (jointly with DS, HL, MA, O)**
TT 43.1–43.6	Tue	14:00–15:45	H 2053	**Superconductivity: Fe-based Superconductors – 122**
TT 44.1–44.7	Tue	14:00–15:45	H 3005	**Correlated Electrons: Quantum-Critical Phenomena – Experiments**
TT 45.1–45.8	Tue	14:00–16:00	H 3010	**Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 3 (jointly with DY)**
TT 46.1–46.7	Tue	14:00–15:45	A 053	**Transport: Nanomechanics (jointly with MM)**
TT 47.1–47.7	Tue	14:00–16:00	C 130	**Organic Electronics and Photovoltaics: OPV I (jointly with CPP, HL, O)**
TT 48.1–48.6	Tue	14:30–16:00	BH-N 334	**Quantum Chaos (jointly with DY)**
TT 49.1–49.6	Tue	14:00–15:45	MA 004	**Frontiers of Electronic Structure Theory: Charge and Spin Dynamics (jointly with O, HL)**
TT 50.1–50.20	Tue	18:15–21:00	Poster A	**Graphene (organized by O)**
TT 51.1–51.5	Wed	9:30–12:15	H 0104	**Focus Session: Electric Power Applications of Superconductivity**

TT 52.1–52.11	Wed	9:30–12:30	H 2053	**Superconductivity: Fe-based Superconductors – FeSe and others**
TT 53.1–53.1	Wed	9:30– 9:45	H 3005	**Superconductivity: Vortex Physics**
TT 54.1–54.5	Wed	9:45–11:00	H 3005	**Superconductivity: Heterostructures**
TT 55.1–55.13	Wed	9:30–13:00	H 3010	**Low-Dimensional Systems: 2D – Theory**
TT 56.1–56.14	Wed	9:30–13:15	A 053	**Correlated Electrons: Quantum-Critical Phenomena – Theory**
TT 57.1–57.5	Wed	11:30–12:45	H 3005	**Transport: Fluctuations and Noise (jointly with CPP, DY)**
TT 58.1–58.8	Wed	9:30–11:30	H 0110	**Spincaloric Transport I (jointly with MA)**
TT 59.1–59.13	Wed	9:30–13:00	EB 107	**Multiferroics I (jointly with DF, DS, KR, MA)**
TT 60.1–60.13	Wed	9:30–13:00	C 130	**Organic Electronics and Photovoltaics: OPV II (jointly with CPP, HL)**
TT 61.1–61.11	Wed	10:30–13:30	MA 004	**Frontiers of Electronic Structure Theory: Organics and Materials (jointly with O, HL)**
TT 62.1–62.9	Wed	10:30–13:00	MA 041	**Graphene: Dynamics (jointly with O, HL)**
TT 63.1–63.8	Wed	9:30–11:30	ER 270	**Topological Insulators: Theory (jointly with HL, DS, MA, O)**
TT 64.1–64.8	Wed	11:00–13:00	EW 202	**Quantum Information Systems: Mostly Concepts (jointly with HL)**
TT 65.1–65.15	Wed	15:00–19:15	H 0104	**Low-Dimensional Systems: 1D – Theory**
TT 66.1–66.15	Wed	15:00–19:15	H 2053	**Superconductivity: Tunneling, Josephson Junctions, SQUIDs**
TT 67.1–67.10	Wed	15:00–17:45	H 3005	**Correlated Electrons: f-Electron Systems**
TT 68.1–68.11	Wed	15:00–18:15	H 3010	**Correlated Electrons: (General) Theory 1**
TT 69.1–69.15	Wed	15:00–19:00	A 053	**Other Low Temperature Topics: Cold Atomic Gases**
TT 70.1–70.5	Wed	18:00–19:15	H 3005	**Correlated Electrons: Spin Systems and Itinerant Magnets – Chiral Magnets (jointly with MA)**
TT 71.1–71.80	Wed	15:00–18:00	Poster B	**Correlated Electrons: Poster Session**
TT 72.1–72.21	Wed	15:00–18:00	Poster B	**Low-Dimensional Systems: Poster Session**
TT 73.1–73.8	Wed	15:00–17:00	H 0110	**Spincaloric Transport II (jointly with MA)**
TT 74.1–74.5	Wed	15:00–17:45	H 1012	**Focus Session: Ultra-Fast Magnetism under Electronic Nonequilibrium Conditions (organized by MA)**
TT 75.1–75.13	Wed	15:00–18:50	EB 107	**Multiferroics II (jointly with DF, DS, KR, MA)**
TT 76.1–76.8	Wed	16:45–18:45	ER 270	**Graphene: Applications, Luminescence, and Spin Relaxation (jointly with HL, O)**
TT 77.1–77.6	Wed	15:00–16:30	ER 270	**Topological Insulators: Structure and Electronic Structure (jointly with HL, DS, MA, O)**
TT 78.1–78.5	Wed	11:45–13:00	ER 270	**Topological Insulators: Transport (jointly with HL, DS, MA, O)**
TT 79.1–79.13	Wed	15:00–18:30	MA 004	**Frontiers of Electronic Structure Theory: Optical Excitation (organized by O)**
TT 80.1–80.10	Wed	15:00–17:45	MA 005	**2D Materials Beyond Graphene: TMDCs, Silicene and Relatives (organized by O)**
TT 81.1–81.10	Wed	18:15–21:00	Poster A	**Electronic Structure Theory: Many-Body Effects (organized by O)**
TT 82.1–82.7	Wed	18:15–21:00	Poster A	**Electronic Structure Theory: General, Method Development (organized by O)**
TT 83.1–83.7	Wed	18:15–21:00	Poster A	**Graphene: Adsorption, Intercalation and Doping (organized by O)**
TT 84.1–84.9	Thu	9:30–13:15	H 0104	**Focus Session: Nanoscopic Superconducting Heterostructures**
TT 85.1–85.6	Thu	9:30–11:15	H 2053	**Superconductivity: Higgs Modes in Condensed Matter and Quantum Gases (jointly with DY, MA, O)**
TT 86.1–86.13	Thu	9:30–13:00	H 3005	**Correlated Electrons: (General) Theory 2**
TT 87.1–87.6	Thu	9:30–11:00	H 3010	**Low-Dimensional Systems: Molecular Conductors (jointly with CPP, HL, MA, O)**
TT 88.1–88.5	Thu	9:30–10:45	A 053	**Transport: Carbon Nanotubes**
TT 89.1–89.8	Thu	11:00–13:00	A 053	**Transport: Quantum Dots, Quantum Wires, Point Contacts 1 (jointly with HL)**
TT 90.1–90.6	Thu	11:30–13:00	H 3010	**Low-Dimensional Systems: Topological Order 1 (jointly with DS, HL, MA, O)**

TT 91.1–91.6	Thu	11:30–13:00	H 2053	**Superconductivity: (General) Theory 1**
TT 92.1–92.10	Thu	9:30–12:00	EB 202	**Topological Insulators I (jointly with MA, DS, HL, O)**
TT 93.1–93.13	Thu	9:30–13:00	H 0111	**Graphen (organized by DS)**
TT 94.1–94.8	Thu	9:30–11:30	H 0112	**Spin-Dependent Transport Phenomena I (organized by MA)**
TT 95.1–95.9	Thu	10:00–12:30	ER 164	**Spintronics: Mobile Electrons and Holes (jointly with HL, MA)**
TT 96.1–96.10	Thu	10:30–13:15	MA 004	**Frontiers of Electronic Structure Theory: 2D TMDC and Excitonic Effects (organized by O)**
TT 97.1–97.10	Thu	10:30–13:00	MA 041	**Graphene: Structure (jointly with O, HL)**
TT 98.1–98.7	Thu	15:00–18:15	H 0104	**Focus Session: Visualization of Heavy Fermion Formation through Scanning Tunneling Microscopy**
TT 99.1–99.11	Thu	15:00–18:00	H 2053	**Superconductivity: (General) Theory 2**
TT 100.1–100.13	Thu	15:00–18:30	H 3005	**Correlated Electrons: Other Materials**
TT 101.1–101.13	Thu	15:00–18:30	H 3010	**Low-Dimensional Systems: Topological Order 2 (jointly with DS, HL, MA, O)**
TT 102.1–102.12	Thu	15:00–18:30	A 053	**Transport: Quantum Dots, Quantum Wires, Point Contacts 2 (jointly with HL)**
TT 103.1–103.54	Thu	15:00–18:00	Poster B	**Transport: Poster Session**
TT 104.1–104.11	Thu	15:00–17:45	EB 202	**Topological Insulators II (jointly with MA, DS, HL, O)**
TT 105.1–105.8	Thu	15:00–17:00	ER 164	**Quantum Information Systems: Si Vacancies and NV Centers (jointly with HL)**
TT 106.1–106.13	Thu	15:00–18:30	MA 004	**Frontiers of Electronic Structure Theory: Many-Body Effects, Methods (organized by O)**
TT 107.1–107.13	Thu	15:00–18:15	MA 041	**Graphene: Electronic Structure (jointly with O, HL)**
TT 108.1–108.11	Thu	15:00–18:00	H 0112	**Spin-Dependent Transport Phenomena II (organized by MA)**
TT 109.1–109.10	Fri	9:30–12:15	H 0104	**Transport: Majorana Fermions (jointly with DS, HL, MA, O)**
TT 110.1–110.10	Fri	9:30–12:15	H 2053	**Superconductivity: Fe-based Superconductors – Theory**
TT 111.1–111.10	Fri	9:30–12:15	H 3005	**Correlated Electrons: Quantum Impurities, Kondo Physics**
TT 112.1–112.9	Fri	9:30–12:00	H 3010	**Correlated Electrons: (General) Theory 3**
TT 113.1–113.7	Fri	9:30–12:00	C 130	**Organic Electronics and Photovoltaics: Devices (jointly with CPP, HL)**
TT 114.1–114.10	Fri	9:30–12:15	H 0110	**Transport: Molecular Electronics (jointly with CPP, HL, MA, O)**
TT 115.1–115.13	Fri	9:30–13:15	H 2032	**Metallic Nanowires on the Atomic Scale (jointly with DS, O)**
TT 116.1–116.9	Fri	9:30–12:00	EB 202	**Spintronics (incl. Quantum Dynamics) (jointly with MA, HL)**
TT 117.1–117.9	Fri	10:30–12:45	MA 041	**Graphene: Intercalation (jointly with O, HL)**

Annual General Meeting of the Low Temperature Physics Division

Thursday 18:45–20:00 Room H 3005

TT 1: Tutorial: Nonequilibrium Renormalization Group Methods

This tutorial provides introductions to three essentially analytic renormalization-group-like approaches to the quantum many-body problem in non-equilibrium. They constitute versatile tools to investigate driven steady states as well as the nonequilibrium dynamics of correlated systems in different fields of growing interest such as, e.g., meso- and nanoscopic solid-state systems, as well as cold atomic gases.

Organizer: Volker Meden (RWTH Aachen)

Time: Sunday 16:00–18:15 Location: H 0110

Introductory Remarks

Tutorial TT 1.1 Sun 16:05 H 0110

From Lunar Motion to Real Time Evolution of Quantum Many-Body Systems — •Stefan Kehrein — Institute for Theoretical Physics, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

While studying the real time evolution of quantum many-body systems is a fairly new topic in physics, the real time evolution of classical systems is an old one. In fact, this topic goes back to the very beginning of classical mechanics, namely its application to celestial mechanics. One of the important lessons learned in this classical setting is that naive application of perturbation theory can lead to secular terms in time which quickly invalidate the expansion. This observation gave rise to the development of canonical perturbation theory with much improved convergence properties.

In this lecture I will show how similar progress can be made for the calculation of the real time evolution of quantum systems by using unitary perturbation theory [1,2,3]. In addition, this approach permits one to deal with models with a nontrivial renormalization flow and to see how this affects the real time dynamics away from equilibrium.

[1] A. Hackl and S. Kehrein, Phys. Rev. B **78**, 092303 (2008)
[2] A. Hackl and S. Kehrein, J. Phys. C **21**, 015601 (2009)
[3] F. Essler, S. Kehrein, S. Manmana, and N. Robinson, Phys. Rev. B **89**, 165104 (2014)

5 min. break

Tutorial TT 1.2 Sun 16:50 H 0110

Functional Renormalization Group Approach to Nonequilibrium Transport through Mesoscopic Systems — •Severin Georg Jakobs — Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany

The transport properties of quantum dots and wires are strongly influenced by correlation effects like the Kondo effect or Luttinger liquid behavior. The theoretical description of these effects requires methods beyond plain perturbation theory or mean-field theory. In the last decade, the functional renormalization group (fRG) has been used extensively and successfully to investigate such situations. It is applicable if the interaction on the dot is weak to intermediate compared to the hybridization with the leads. This makes the method complementary to the real-time RG which applies to the opposite regime and which is described in the tutorial by Herbert Schoeller. The particular formulation of the fRG in the framework of Keldysh formalism allows to study time-dependent and steady-state nonequilibrium situations. In this tutorial I introduce the basic concepts of that method and discuss the choice of appropriate flow parameters. I discuss examples for steady-state transport at finite bias voltage and for the time-dependent transient regime.

5 min. break

Tutorial TT 1.3 Sun 17:35 H 0110

Real-Time RG: Nonequilibrium Properties of Open Quantum Systems — •Herbert Schoeller — Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany — JARA-Fundamentals of Future Information Technology

A tutorial introduction is presented for the description of nonequilibrium properties of few-level quantum sytems coupled to reservoirs as e.g. realized by quantum dot, spin boson or Kondo models. Within a quantum field theoretical framework in Liouville space it is shown how formally exact kinetic equations can be derived which can be systematically studied in terms of an effective Liouvillian. By using special resummation techniques via self-consistent perturbation theory and renormalization group methods it is shown how the time evolution and the stationary state can be studied in a nonequilibrium set-up. Various applications in the weak and strong coupling limit are presented.

TT 2: Tutorial: Ferroics (organized by DF)

This tutorial introduces the field of domain and domain-wall engineering, key concepts and materials, and launches our 3-days focus on ferroic domain walls. The tutorial will provide a forum for non-specialists to get informed / involved and, at the same time, aims at inspiring topical discussions to stimulate a vivid scientific exchange during the following Sypmosium (SYDW), the three Focus Sessions and a Poster Session.

Organizers: Elisabeth Soergel (Universität Bonn) and Dennis Meier (ETH Zürich)

Time: Sunday 16:00–18:30 Location: H 0107

Tutorial TT 2.1 Sun 16:00 H 0107

Fundamentals of ferroelectric materials — •Susan Trolier-McKinstry — Penn State University, University Park, PA, USA

This tutorial will cover the fundamental phenomena that underpin the field of ferroelectricity, with an emphasis on the relationship between crystal structure and the allowed domain states. An introduction will be made to ferroelectricity, pyroelectricity, piezoelectricity, and the origins of the dielectric response. The crystal structures of key materials, including perovskites, $LiNbO_3$, the tungsten bronzes, and polymer ferroelectrics will be introduced, along with the link between the loss of symmetry elements and the allowed domain states. The tutorial will conclude with an introduction to the movement of domain walls, and the influence that this has on the properties of ferroelectric materials.

Tutorial TT 2.2 Sun 16:50 H 0107

Domain walls in multiferroics as functional oxide interfaces — •Manfred Fiebig — Department of Materials, ETH Zürich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland

The functionality of any ferroic material depends on its domains. Consequently, their shape and manipulation in external fields are of major research interest. In compounds uniting magnetic and electric order in the same phase, the magnetoelectric coupling on the level of the domains is, however, largely unexplored. For such so-called multiferroics it is therefore not known how exactly electric or magnetic fields affect the multiferroic domains and their walls. In my talk I will discuss this issue and focus on the influence of the multiferroic order on the ferroelectric state and its domain walls. Examples I will include are: (i) multiferroics with geometric ferroelectricity such as hexagonal $YMnO_3$ where the domain walls exhibit anisotropic conductance and can therefore be regarded as "tunable oxide interfaces"; (ii) multi-

ferroics with magnetically induced ferroelectricity such as $MnWO_4$ or $TbMnO_3$ where the electric polarization within the wall is expected to rotate instead of passing through zero, as in conventional displacive ferroelectrics; (iii) multiferroics with strain-induced ferroelectricity like $SrMnO_3$ where the interplay of strain and oxygen vacancies leads to polar state in which domain walls act as insulating boundaries to the conducting domains.

Tutorial TT 2.3 Sun 17:40 H 0107

Ferroelastic templates for multiferroic domain boundaries — •Ekhard Salje — University of Cambridge, Cambridge, UK

The field of Domain Boundary Engineering is introduced. Ferroelastic domain pattern are derived and their dynamical behaviour is deducted from experimental observations and computer simulations. It is then shown that twin boundaries are particularly easily modified to possess functional properties that do not exist in the bulk. Such functional properties include (super-) conductivity, ferroelectricity, and ferromagnetism. In addition, chemical mixing inside domain walls can generate novel chemical compounds. This effect is refereed to as 'Chemical Mixing in Confined Spaces'. Functionalities often generate chiralities and vortex structures in domain boundaries. It is shown that chirality (in order parameter space) leads to Bloch lines and vortex points as one- and zero-dimensional domain walls embedded in two-dimensional ferroelastic domain walls and are hence walls in walls. Examples in $CaTiO_3$ and $SrTiO_3$ are discussed.

[1] E.K.H. Salje, Ferroelastic Materials, Annual Review of Materials Research, 42, 265-283 (2012)
[2] E.K.H. Salje and K.A. Dahmen, Crackling Noise in Disordered Materials, Annual Review of Condensed Matter Physics, 5, 233-254 (2014)
[3] E.K.H. Salje, Multiferroic Domain Boundaries as Active Memory Devices: Trajectories Towards Domain Boundary Engineering, Chem. Phys. Chem., 11, 940-950 (2010)
[4] D.D. Viehland and E.K.H. Salje, Domain boundary-dominated systems: adaptive structures and functional twin boundaries, Advances in Physics, 63, 267-326 (2014)

TT 3: Tutorial: Density Functional Theory: A Computational Path to Interesting Spin-Textures and Novel Skyrmions (organized by MA)

Organizer: St. Blügel (FZ Jülich)

Ferromagnetic materials are important constituents of many modern hi-tech devices. In the last years one became however aware that non-collinear spin-textures could revolutionize spintronics. The focus of attention is on the spin-orbit interaction in magnetic solids with lack of inversion symmetry, that give rise to magnetic structures of particular winding sense and can lead to the formation of topological magnetization solitons, so-called magnetic skyrmions. These are then new functional magnetic units with interesting dynamical and novel spin-dependent transport properties. Density functional theory is the most powerful theoretical approach providing microscopic inside into the various magnetic interactions and spin-dependent transport properties, which is an important requisite for the design of materials and the analysis of experiments. While density function theory is practised widely, in this field new concepts and tools are coming into play. These will be introduced with the motivation that experimentalists can follow what we really calculate, what we can do, which assumption are made and how theory papers in this field can be interpreted and theory students might get some insight into this modern methodology, widening their scope or applying them to their own problems. After a brief introduction, the first tutorial focusses on the conceptual foundation of the relativistic, spin-dependent density functional theory, the second on the formation of new magnetic ground states and the third on spin-dependent transport properties.

Time: Sunday 16:00–18:30 Location: H 1012

Introductory Remarks

Tutorial TT 3.1 Sun 16:05 H 1012

Introduction to Spin-Density-Functional Theory — •Nicole Helbig — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

Density functional theory is the most powerful framework for a microscopic analysis of electronic properties of real solids. Spin-density-functional theory (spin-DFT) extends the density functional theory framework to allow for the description of magnetic systems, possibly in the presence of an external magnetic field. In this tutorial we introduce this subject from an elementary point of view and discuss the theoretical background of spin-DFT in both its collinear and non-collinear versions. Approximations for the exchange-correlation energy, which are necessary for practical applications, are also introduced. We give examples for calculations of different magnetic structures within spin-DFT and discuss how the theoretical results compare to experiments.

Tutorial TT 3.2 Sun 16:50 H 1012

Determining chiral magnetism from density functional theory — •Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Spin-orbit interaction in magnetic solids with bulk or structure inversion-asymmetry leads to the Dzyaloshinskii-Moriya interaction [1]. This magnetic interaction is a source of chiral magnetism and can subsequently lead to magnetic skyrmions – topological magnetization solitons – that may open a completely new vista to spintronics. A crucial issue is to find magnetic materials and ultra-thin films that combine the right properties such that these skyrmions can be formed. Density functional theory is a theoretical framework that permits the calculation of magnetic properties of materials from first-principles and is as such a tool for the analysis of experiments, for providing understanding of the magnetic interaction and for the design of the proper materials. In this endeavor your help is requested, many more *ab initio* calculations and experiments are needed. In this tutorial I explain concepts used to find these complex magnetic phases. The tutorial is conceptualized such that experimentalists can follow what we really calculate and what we can do and which assumptions are made, and theory students might get some insight into our methodology [2]. Examples are discussed mostly from the field of thin films [3].

[1] M. Bode *et al.*, Nature **447**, 190 (2007).
[2] see for example `www.juDFT.de`
[3] S. Heinze *et al.*, Nature Physics **7**, 713 (2011).

10 min. break

Tutorial TT 3.3 Sun 17:45 H 1012

Magneto-transport properties in spiralling spin textures — •Yuriy Mokrousov — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Spin-dependent transport properties in chiral magnets are currently of great interest both experimentally and theoretically. In this respect the skyrmion lattices comprised of topologically non-trivial whirls of magnetization which are typically stabilized at small magnetic field in the vicinity of the magnetic transition temperature are particularly

intensively studied in B20 compounds. The Hall signal measured in these systems contains two topology-driven contributions due to the topological Hall effect (THE) and the anomalous Hall effect (AHE). It can be shown that the THE and AHE are a consequence of the Berry phases which electrons pick up in real and reciprocal spaces, respectively, while the so-called mixed Berry phases due to coupled dynamics in real and reciprocal space would give rise to a magnetic interaction which favors the chirality of the magnetization and gives rise to the skyrmion lattice - the Dzyaloshinskii-Moriya interaction (DMI). In my talk I will show how first principles methods can be used to justify the validity of the Berry phase concepts, as well as estimate and understand the physics of transport properties and DMI in skyrmion phase of complex materials. Moreover, I will try to convey a point that advanced material-specific modelling is a unique tool, which can be used to explore the emergent field of magneto-transport in nanometer-scale non-collinear textures.

TT 4: Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 1 (jointly with DY)

Time: Monday 9:30–13:00 Location: H 0104

Topical Talk TT 4.1 Mon 9:30 H 0104

Entanglement in the Many-Body Localized Phase and Transition — •Jens H. Bardarson — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The study of entanglement, both in eigenstates and its evolution after quenches, has been instrumental in advancing our understanding of many-body localized phases—the interacting analogs of the Anderson insulator. In this talk I will discuss in detail three observations related to the entanglement properties of many-body localized systems: (i) A global quench within the many-body localized phase gives rise to a slowly (logarithmically) increasing entanglement entropy. This is due to interaction induced dephasing that is absent in the Anderson insulator and therefore serves as a unique signature of the many-body localized phase. (ii) A local quench from an eigenstate leads to an extensive increase in the entanglement entropy only at the many-body localization transition itself. And (iii) at the many-body localization transition the distribution of entanglement entropies becomes extensively broad, while it vanishes both in the extended metallic phase and in the localized phases. The width of the entanglement distribution, like the long time limit of the local quench, is therefore a useful diagnostic for a many-body localization transition. I explicitly demonstrate how all these features are observed in microscopic spin chain models of many-body localization, and, in particular, discuss how they can be used to detect a many-body mobility edge.

[1] JHB, Pollmann, and Moore, PRL **109**, 017202 (2012).
[2] Kjall, JHB, and Pollmann, PRL **113**, 107204 (2014).

TT 4.2 Mon 10:00 H 0104

Dynamics of competing orders in YBCO triggered by ultrafast light pulses — •Junichi Okamoto, Robert Höppner, Beilei Zhu, and Ludwig Mathey — Institute for Laser Physics, University of Hamburg, Hamburg, Germany

In the emerging field of optically driven strongly correlated systems, laser-excited high-T_c cuprates are one of the most fascinating topics. In equilibrium, the underdoped region of high-T_c cuprates exhibit various competing orders, e.g., stripes, density-waves and superconductivity. In this talk, we will explore the possibility of optically controlling such competing orders. In particular, we will focus on the underdoped region of YBCO, where d-wave superconductivity and charge-density waves coexist. We will present preliminary results of numerical simulations of optically driven competing orders in the material.

TT 4.3 Mon 10:15 H 0104

Ultrafast dynamics in $CeTe_3$ near the pressure-induced charge-density-wave transition — Jonas Tauch[1], Hanjo Schäfer[1,2], Manuel Obergfell[1], Jure Demsar[1,2,3], Paula Giraldo[4], Ian R. Fisher[4], and •Alexej Pashkin[1,5] — [1]Department of Physics and Center for Applied Photonics, University of Konstanz, Germany — [2]Institute of Physics, Ilmenau University of Technology, Germany — [3]Institute of Physics, Johannes Gutenberg-University Mainz, Germany — [4]Geballe Laboratory for Advanced Materials and Department of Applied Physics, Stanford University, USA — [5]Helmholtz-Zentrum Dresden-Rossendorf, Germany

Femtosecond pump-probe spectroscopy is an efficient tool for studying ultrafast dynamics in strongly correlated electronic systems, in particular, compounds with a charge-density-wave (CDW) order. Application of external pressure often leads to a suppression of a CDW state due to an impairment of the Fermi surface nesting.

We combine time-resolved optical spectroscopy and diamond anvil cell technology to study electron and lattice dynamics in tri-telluride compound $CeTe_3$. Around pressures of 4 GPa we observe a gradual vanishing of the relaxation process related to the recombination of the photoexcited quasiparticles. The coherent oscillations of the phonon modes coupled to the CDW order parameter demonstrate even more dramatic suppression with increasing pressure. These observations clearly indicate a transition into the metallic state of $CeTe_3$ induced by the external pressure.

TT 4.4 Mon 10:30 H 0104

Mechanism of Ultrafast Relaxation of a Photo-Carrier in Antiferromagnetic Spin Background — •Lev Vidmar — University of Munich, Germany

Understanding of relaxation dynamics in correlated condensed-matter systems is vital for identification of dominant couplings in pump-probe experiments, as well as for designing setups where ordered phases are manipulated using external fields.. In many cases, phonons represent an important relaxation channel, however, in two-dimensional systems with antiferromagnetic correlations, this relaxation channel may not be the dominant one [1]. By applying state-of-the-art numerical simulations of the t-J model [2] we show that the relaxation due to coupling to antiferromagnetic spin excitations can be very fast [3]. We show that the key relaxation mechanism at very short times corresponds to the creation of high-energy antiferromagnetic excitations in the close proximity of the photo-excited holes. Such a mechanism enables an energy transfer of more than 1 eV on a 10 femtosecond time scale.

[1] L. Vidmar, J. Bonca, T. Tohyama, and S. Maekawa, Phys. Rev. Lett. 107, 246404 (2011).
[2] M. Mierzejewski, L. Vidmar, J. Bonca, and P. Prelovsek, Phys. Rev. Lett. 106, 196401 (2011).
[3] D. Golez, J. Bonca, M. Mierzejewski, and L. Vidmar, Phys. Rev. B 89, 165118 (2014).

TT 4.5 Mon 10:45 H 0104

Pattern formation in non-equilibrium correlated electronic systems — •Pedro Ribeiro[1], Andrey Antipov[2], and Alexey Rubtsov[1] — [1]Russian Quantum Center, Business-center "Ural", Novaya street 100A, Skolkovo village, Odintsovo district, Moscow area, 143025 Russia — [2]Department of Physics University of Michigan, Randall Laboratory, 450 Church Street, Ann Arbor, MI 48109-1040

Strong non-equilibrium conditions eventually drive a system away from its linear response regime, deeply affecting the properties of the underlying equilibrium phase. A well known example is the Rayleigh-Bernard convection arising for classical fluids that develop convection rolls of a specific wave-length. We report on recent results regarding effects of large bias voltages applied across a half-filled Hubbard chain. At equilibrium this system shows a charge gap and strong antiferromagnetic correlations. We show that out of equilibrium the wavevector maximizing the spin-susceptibility shifts from its equilibrium antiferromagnetic value $q = \pi$ as a function of the applied voltage and temperature. We describe a rich set of phases induced by the interplay between electron-electron interactions and non-equilibrium conditions. Some of phases found are examples of non-equilibrium-induced spacial pattern formation. We comment on the properties and stability of these phases. Finally we argue that, although no symmetry breaking arises in the 1D system, these results suggest that a spatially modulated charge gap may be observed experimentally by STM in engineered atomic chains and nano-wires.

TT 4.6 Mon 11:00 H 0104

Time-dependent Gutzwiller wave function for the Hubbard model in nonequilibrium — •Marcus Kollar[1] and Christian Gramsch[1,2] — [1]Theoretische Physik III, Universitität Augsburg — [2]I. Institut für Theoretische Physik, Universität Hamburg

In previous studies the time-dependent Gutzwiller wave function (GWF) has been applied to the fermionic Hubbard model in nonequilibrium [1], using the Gutzwiller approximation which is known to become exact in the limit of infinite lattice dimension. As an alternative, we employ the variational formalism for the GWF which applies in arbitrary dimensions, recovering the dynamics obtained in Ref. [1]. We present results for the one-dimensional Hubbard model, for which exact evaluations of the GWF are available. In particular we find that the GWF captures the transient momentum distribution on short timescales [2].

[1] M. Schiró and M. Fabrizio, Phys. Rev. Lett. **105**, 076401 (2010).
[2] S. A. Hamerla and G. S. Uhrig, Phys. Rev. B **87**, 064304 (2013).

15 min. break.

TT 4.7 Mon 11:30 H 0104

Nonequilibrium dynamics of screening in the extended Hubbard model — •Denis Golež and Philipp Werner — University of Fribourg

We will present a study of the non-equilibrium dynamics in the extended Hubbard model on the square lattice using time-dependent extended dynamical mean-field theory. The short-time effect of the dynamical screening due to the photo-doping is the reduction of the effective static interaction. On the same time scale the fully screened interaction is transformed from the single to double mode structure due to photo-doped charge carriers. At longer times the the dynamical screening enhance the relaxation dynamics.

TT 4.8 Mon 11:45 H 0104

Continuous monitoring of a quantum many-body system — •Thomas Kiendl[1], Vinay Ramasesh[2], Shay Hacohen-Gourgy[2], Irfan Siddiqi[2], and Florian Marquardt[1] — [1]Institut for Theoretical Physics, Universität Erlangen-Nürnberg, Staudtstraße 7, D-91058 Erlangen, Germany — [2]QNL, University of California, Berkeley

At the heart of quantum mechanics lies the fact that a measurement causes back-action on the system itself. A prominent example is the quantum Zeno effect. Observing a system continuously with a large measurement strength freezes the system's dynamics. We explore how such phenomena transfer to a quantum many-body system, employing a chain of qubits as an experimentally relevant example. Using the concept of weak, continuous measurements we investigate new timescales caused by continuous monitoring of the chain. In this context, we present new results on relaxation dynamics and thermalization for both integrable and non-integrable Hamiltonians.

TT 4.9 Mon 12:00 H 0104

Influence of quadrupolar interactions in the anisotropic central spin model — •Johannes Hackmann and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für theoretische Physik II, 44221 Dortmund, Germany

We have investigated spin noise in an ensemble of semiconductor quantum dots (QDs). A single electron (or hole) doped QD is described by the anisotropic central spin model. Additionally, the quadrupole moments of the nuclei couple to strain induced electric fields in the QD. We investigated the influence of these quadrupolar couplings on the central spin dynamics, that are calculated via the correlation functions $\langle S^z(t)S^z\rangle$ and $\langle S^z(\omega)S^z\rangle$. We demonstrate that our results are in good agreement with recent experiments and show that quadrupolar interactions have a large impact on measurements on hole doped QDs, while they almost are negligible for the case of electron doped QDs.

TT 4.10 Mon 12:15 H 0104

The generic fixed point model for pseudo-spin-1/2 quantum dots in nonequilibrium: Spin-valve systems with compensating spin polarizations — Stefan Göttel[1,2], Frank Reininghaus[1,2], and •Herbert Schoeller[1,2] — [1]Institute for Theory of Statistical Physics, RWTH Aachen — [2]JARA-Fundamentals of Future Information Technology

We study a pseudo-spin-1/2 quantum dot in the cotunneling regime close to the particle-hole symmetric point. For a generic tunneling matrix we find a generic fixed point with interesting nonequilibrium properties, characterized by effective reservoirs with compensating spin orientation vectors weighted by the polarizations and the tunneling rates. At large bias voltage we study the magnetic field dependence of the dot magnetization and the current. The fixed point can be clearly identified by analysing the magnetization of the dot. We characterize in detail the universal properties for the case of two reservoirs.

TT 4.11 Mon 12:30 H 0104

First order dynamical phase transitions — •Elena Canovi[1], Philipp Werner[2], and Martin Eckstein[1] — [1]Max Planck Research Department for Structural Dynamics, University of Hamburg (CFEL), Building 99, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland

Recently, dynamical phase transitions have been identified based on the non-analytic behavior of the Loschmidt echo in the thermodynamic limit [1]. By introducing conditional probability amplitudes, we show how dynamical phase transitions can be further classified, both mathematically, and potentially in experiment. This leads to the definition of first-order dynamical phase transitions. Furthermore, we develop a generalized Keldysh formalism which allows to use nonequilibrium dynamical mean-field theory to study the Loschmidt echo and dynamical phase transitions in high-dimensional, non-integrable models. We find dynamical phase transitions of first order in the Falicov-Kimball model and in the Hubbard model.

[1] Heyl et al., Phys. Rev. Lett. 110, 135704 (2013).

TT 4.12 Mon 12:45 H 0104

Holography of the toric code — •Johannes Oberreuter and Stefan Kehrein — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

Dynamics of quantum-many-body systems at weak coupling can be effectively described by quasi-particles. At strong coupling, the quasiparticle picture breaks down. Instead of resorting to numerics one can use a duality, which relates strongly coupled (conformal) field theories to classical, weakly coupled (Einstein) gravity in one dimension higher, the so-called gauge/gravity duality or AdS/CFT-correspondence. The correlation functions of the field theory can then in principle be computed from a calculation in classical gravity. The correspondence, however, in general only applies to conformal field theories and it is difficult to describe systems of interest in condensed matter theory. The observation of similarities in calculating the entanglement entropy in AdS/CFT and in MERA, a particular tensor network of a quantum state, has led to the conjecture that MERA might be a discrete version of the gauge-gravity duality. It is in principle possible to represent any quantum state in MERA. We investigate this idea in the toric code, where the representation is known exactly [1] and comment on the non-generic behaviour of this model including its dynamics.

[1] M. Aguado, G. Vidal, Phys. Rev. Lett. 100, 070404 (2008).

TT 5: Correlated Electrons: Spin Systems and Itinerant Magnets – Frustrated Magnets 1 (jointly with MA)

Time: Monday 9:30–13:00 Location: H 0110

TT 5.1 Mon 9:30 H 0110

Investigation into the Magnetic Properties of Pyrochlore-type Rare-Earth Hafnates — •Jung Hwan Chun, Reinhard K. Kremer, and Chengtian Lin — MPI for Solid State Research, Stuttgart, Germany

Cubic rare-earths transition metal pyrochlores with composition $R_2TM_2O_7$ have attracted broad attention because of their unusual magnetic ground state properties related to geometrical frustration of the pyrochlores lattice. So far, the investigation focused mainly on $3d$ and $4d$ transition metal systems. The magnetic properties of rare-earths $5d$ TM pyrochlores are comparatively less well studied. Here we report on the single-crystal growth and the magnetic properties of some rare-earth hafnates (R =Nd, Gd, Dy; TM = Hf) of composition $R_2Hf_2O_7$. $Nd_2Hf_2O_7$ and $Gd_2Hf_2O_7$ crystallize with the cubic pyrochlores structure whereas diverging reports on the structure of $Dy_2Hf_2O_7$ are available in literature. Crystals of $R_2Hf_2O_7$ have been grown and their structural and magnetic properties have been investigated. Our investigations confirm $Nd_2Hf_2O_7$ and $Gd_2Hf_2O_7$ to crystallize in the cubic pyrochlores structure. Antiferromagnetic ordering below $\sim$0.5 K has been observed by magnetic susceptibility and heat capacity measurements for both compounds.

TT 5.2 Mon 9:45 H 0110

Finite-temperature dynamics of a highly frustrated quantum spin ladder — •Andreas Honecker[1] and Bruce Normand[2] — [1]LPTM, Université de Cergy-Pontoise, France — [2]Renmin University of China, Beijing

Highly-frustrated magnets are characterized by a (nearly) flat one-triplet excitation band at zero temperature. Little is known from theoretical studies about the temperature-dependence of this single-particle dispersion and less still concerning multi-particle dynamics at finite temperature. Experimentally, inelastic neutron scattering studies of low-dimensional frustrated systems such as $SrCu_2(BO_3)_2$ require an interpretation of the thermal evolution of scattering intensities. We investigate these issues using the example of a highly frustrated spin-1/2 ladder. We find that single- and many-particle excitations persist as sharp spectral features in the dynamic structure factor to surprisingly high and even infinite temperatures. In addition, in a relevant parameter regime low-lying excitations give rise to an anomalously rapid transfer of spectral weight out of the single-particle band to a wide range of energies.

TT 5.3 Mon 10:00 H 0110

Quantum phases of the frustrated Heisenberg model on the bilayer honeycomb lattice — •Wolfram Brenig[1], Marcelo Arlego[2], and Carlos Lamas[2] — [1]Institute for Theoretical Physics, Technical University Braunschweig, Germany — [2]IFLP - CONICET, Departamento de Física, Universidad Nacional de La Plata, Argentina

We analalyze the spin-1/2 Heisenberg antiferromagnet on the honeycomb bilayer with frustrateing next-nearest neighbor exchange. Using a combination of bond-operators, Schwinger-boson mean field theory, and dimer series expansion we evaluate and compare results for the magnetic quantum phase diagram as a function of the intra(inter) planar couplings $J_{1,2}(J_\perp)$. Evidence for both, magnetically ordered and disordered phases will be presented from results for the ground state energy, the spin gap, and real space spin-spin correlation functions. The presence of Néel, dimer, nematic, and non-collinear states will be discussed.

TT 5.4 Mon 10:15 H 0110

Spin dynamics of the bilinear-biquadratic spin-one Heisenberg model on the triangular lattice — Annika Völl and •Stefan Wessel — Institut für Theoretische Festkörperphysik, RWTH Aachen University, Germany

We study thermodynamic properties as well as the dynamical spin and quadrupolar structure factors of the O(3)-symmetric spin-1 Heisenberg model with bilinear-biquadratic exchange interactions on the triangular lattice. Based on a sign-problem-free quantum Monte Carlo approach, we access both the ferromagnetic and the ferroquadrupolar ordered, spin nematic phase as well as the SU(3)-symmetric point which separates these phases. Signatures of Goldstone soft-modes in the dynamical spin and the quadrupolar structure factors are identified, and the properties of the low-energy excitations are compared to the thermodynamic behavior observed at finite temperatures as well as to Schwinger-boson flavor-wave theory.

TT 5.5 Mon 10:30 H 0110

Quantum spin liquid in a π flux triangular lattice Hubbard model — •Stephan Rachel[1], Manuel Laubach[2], Johannes Reuther[3], and Ronny Thomale[2] — [1]Technische Universität Dresden — [2]Universität Würzburg — [3]Dahlem Center for Complex Quantum Systems and FU Berlin

We propose the π flux triangular lattice Hubbard model (π-THM) as a prototypical setup to stabilize magnetically disordered quantum states of matter in the presence of charge fluctuations. The quantum paramagnetic domain of the π-THM which we identify for intermediate Hubbard U is framed by a Dirac semi-metal for weak coupling and by 120° Néel order for strong coupling. Generalizing the Klein duality from spin Hamiltonians to tight-binding models, the π-THM maps to a Hubbard model which corresponds to the $(J_H, J_K) = (-1, 2)$ Heisenberg-Kitaev model in its strong coupling limit. The π-THM provides a promising microscopic testing ground for exotic finite-U spin liquid ground states amenable to numerical investigation.

TT 5.6 Mon 10:45 H 0110

Quantum Monte Carlo Study of Long-Range Transverse-Field Ising Models on the Triangular Lattice — •Stephan Humeniuk — Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany

Motivated by recent experiments with a Penning ion trap quantum simulator, we perform Stochastic Series Expansion quantum Monte Carlo simulations of long-range transverse-field Ising models on a triangular lattice for different decay powers α of the interactions. The phase boundary for the ferromagnet is obtained as a function of α. For antiferromagnetic interactions we find that the transverse field stabilizes a clock ordered phase with sublattice magnetization $(M, -\frac{M}{2}, -\frac{M}{2})$ with $M \approx 1$ in a process known as "order by disorder" similar to the nearest neighbour antiferromagnet on the triangular lattice. Connecting the known limiting cases of nearest neighbour and infinite-range interactions, we obtain a semi-quantitative phase diagram. Magnetization curves for the ferromagnet for experimentally relevant system sizes and with open boundary conditions are presented.

TT 5.7 Mon 11:00 H 0110

Spin liquids in kagome antiferromagnets — •Yin-Chen He, Siddhardh Morampudi, and Frank Pollmann — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187, Dresden, Germany

We propose a novel approach to describe critical spin liquids for $S = 1/2$ kagome antiferromagnets. Instead of a physical spin system, we are working on a dual model, which deals with emergent pseudo spin coupled with a compact $U(1)$ gauge field. We show that by fractionalizing the pseudo spins one can construct a class of stable deconfined critical spin liquids. This spin liquid is very different from the traditional ones, e.g., it has two different kinds of gauge field, and cannot simply be reproduced using the traditional spinon parton approach. Further, we show that a simple mean field ansatz yields an exotic critical spin liquid phase, which is described by 16 flavors of Dirac fermions coupled with one $U(1)$ and two Z_2 gauge fields. We also show such critical spin liquid can be the parent state of chiral and Z_2 spin liquids.

15 min. break.

TT 5.8 Mon 11:30 H 0110

$\mathbb{Z}_2$-vortex lattice in the ground state of Kitaev-Heisenberg models — •Maria Daghofer[1], Ioannis Rousochatzakis[2], Ulrich K Rössler[3], and Jeroen van den Brink[3] — [1]nstitut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [3]IFW Dresden, Dresden

In geometrically frustrated magnets, the strongly competing interactions between spins often suppress simple magnetic ordering patterns and clear space for new states of matter supporting rather exotic excitations, for instance, magnetic monopoles as topological excitations of spin-ice states on pyrochlore lattices. The triangular-lattice Heisenberg antiferromagnet also carries topological excitations, $\mathbb{Z}_2$ vortices, which form a $\mathbb{Z}_2$-vortex gas at finite temperatures. Here we show that spin-orbit interaction, introduced via a Kitaev term in the exchange Hamiltonian, causes the vortices to condense into a hexagonal superlattice at zero temperature. This is a new example of a nucleation transition, analogous to the Abrikosov vortex lattices in type-II superconductors, the blue phases in cholesteric liquid crystals, and the skyrmionic lattices observed in B20 chiral helimagnets. As the mechanism relies on the interplay of geometric frustration and orbital anisotropies, such vortex mesophases can materialize as a ground-state property in spin-orbit coupled correlated systems with nearly hexagonal topology, as in triangular or strongly frustrated honeycomb iridates.

TT 5.9 Mon 11:45 H 0110

Magnetic order within Kitaev–Heisenberg model — •Dorota Gotfryd[1] and Andrzej M. Oleś[2,3] — [1]Institute of Theoretical Physics, Warsaw University, Pasteura 5, PL-02093 Warsaw, Poland — [2]Marian Smoluchowski Institute of Physics, Jagiellonian University, prof. S. Łojasiewicza 11, PL-30348 Kraków, Poland — [3]Max-Planck-Institut FKF, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

We present the evolution of energy spectra, spin correlation functions and order parameters for Kitaev–Heisenberg (KH) model on a single hexagon within a cluster mean-field approximation introduced in [1] in order to induce the breaking of SU(2) symmetry. The changes of these quantities are used to determine quantum phase transitions within KH model between the antiferromagnetic, stripe and Kitaev phases. In the quest of seeking physically preferred zigzag phase [2] we investigate the modifications of the phase diagram given by: (*i*) second and third neighbor Heisenberg terms, and (*ii*) anisotripic Ising-like terms added to KH Hamiltonian. We discuss the stability of this phase and possible implications for honeycomb iridates.

This work is supported by the NCN Project No. 2012/04/A/ST3/00331.

[1] A. F. Albuquerque *et al.*, Phys. Rev. B **84**, 024406 (2011).
[2] J. G. Rau *et al.*, Phys. Rev. Lett. **112**, 077204 (2014).

TT 5.10 Mon 12:00 H 0110

Emergent critical phase and Z_6 order in the windmill lattice antiferromagnet — •Peter P Orth[1], Bhilahari Jeevanesan[1], Joerg Schmalian[1], Premala Chandra[2], and Piers Coleman[2] — [1]1Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Center for Materials Theory, Rutgers University, Piscataway, New Jersey 08854, USA

In most systems that exhibit order at low temperatures, the order occurs in the elementary degrees of freedom such as spin or charge. Prominent examples are magnetic or superconducting states of matter. In contrast, emergent order describes the phenomenon where composite objects exhibit longer range correlations. Such emergent order has been suspected to occur in a range of correlated materials. One specific example are spin systems with competing interactions, where long-range discrete order in the relative orientation of spins may occur.

One example is the recently introduced two-dimensional antiferromagnet on the windmill lattice that shows an emergent Z_6 symmetry. The rich ground state phase diagram exhibits intricate spiral and non-coplanar phases. At finite temperature, order by disorder leads to a decoupling of an emergent collective degree of freedom given by the relative phase of spins on different sublattices. Using large scale classical parallel tempering Monte Carlo simulations, we present numerical evidence that the emergent order parameter undergoes a sequence of two Berezinskii-Kosterlitz-Thouless phase transitions that bracket a critical phase. We discuss extensions of this model and physical realizations.

TT 5.11 Mon 12:15 H 0110

The Cu^{2+} mineral szenicsite ($Cu_3(MoO_4)(OH)_4$) - a spin 1/2 J_1-J_2 chain compound with a spin gap — •Stefan Lebernegg[1], Oleg Janson[2], Alexander Tsirlin[3], and Helge Rosner[1] — [1]MPI CPfS, Dresden, Germany — [2]Institute of Solid State Physics, Vienna University of Technology, Austria — [3]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

Low-dimensional quantum magnets attracted high attention because of their exotic magnetic properties and ground states, representing an unrivaled field for challenging our understanding of collective quantum phenomena. These are governed by a complex interplay of quantum fluctuations, exchange interactions and lattice topology, which might result in magnetic frustration suppressing ordering processes. The simplest example of a frustrated system is the 1D J_1-J_2 chain with J_2 being AFM, where J_1 and J_2 are nearest- and next-nearest neighbor exchange couplings, respectively. While for an FM J_1 several materials have been discovered, for J_1 and J_2 both being AFM only very few material realizations have been found so far. In this study, we discuss the Cu^{2+}-mineral szenicsite, $Cu_3(MoO_4)(OH)_4$. A consistent microscopic magnetic model is derived from LSDA+U calculations, which can perfectly reproduce the thermodynamical data. Based on these results, an effective microscopic magnetic model is developed, demonstrating that at low temperatures szenicsite can be described in terms of an AFM J_1-J_2 chain with evidence for alternating J_2 couplings. According to the ratio $J_2/J_1 \sim 0.5$, a small spin gap should be present whose upper limit was estimated with DMRG and ED to be about 2.5 K.

TT 5.12 Mon 12:30 H 0110

The spin-1/2 Heisenberg J_1-J_2 antiferromagnet on the kagome lattice — •Yasir Iqbal[1], Didier Poilblanc[2], and Federico Becca[3] — [1]Institute for Theoretical Physics and Astrophysics, Julius-Maximilian's University of Würzburg, Am Hubland, D-97074, Würzburg, Germany — [2]Laboratoire de Physique Théorique UMR-5152, CNRS and Université de Toulouse, F-31062 Toulouse, France — [3]Democritos National Simulation Center, Istituto Officina dei Materiali del CNR and SISSA-International School for Advanced Studies, Via Bonomea 265, I-34136 Trieste, Italy

We report numerical calculations for the spin-1/2 Heisenberg model in presence of both nearest-neighbor J_1 and next-nearest-neighbor J_2 antiferromagnetic super-exchange couplings. Our approach is based upon Gutzwiller projected fermionic states that represents a flexible tool to describe quantum spin liquids with different properties (e.g., gapless and gapped). We show that, on finite clusters, a gapped $\mathbb{Z}_2$ spin liquid can be stabilized in presence of a finite J_2 super-exchange, with a substantial energy gain with respect to the gapless $U(1)$ Dirac spin liquid. However, this energy gain vanishes in the thermodynamic limit, implying that, at least within this approach, the $U(1)$ Dirac spin liquid remains stable in a relatively large region of the phase diagram. For $J_2/J_1 \gtrsim 0.3$, we find that a magnetically ordered state with $\mathbf{q} = \mathbf{0}$ overcomes the magnetically disordered wave functions, suggesting the end of the putative gapless spin-liquid phase.

TT 5.13 Mon 12:45 H 0110

Topological phases of interacting bosons on the kagome lattice — •Krishanu Roychowdhury[1], Subhro Bhattacharjee[2], and Frank Pollmann[3] — [1]MPIPKS, Dresden — [2]MPIPKS, Dresden — [3]MPIPKS, Dresden

We consider an extended Hubbard model of hard core bosons including nearest-neighbour hopping and long range repulsive interactions on a kagome lattice. The system is an insulator at commensurate fillings of 1/6, 1/3 and 1/2 and can be mapped to different dimer models on the triangular lattice (depending on the filling). We focus on the filling of 1/3, which transforms to a fully packed loop (FPL) model, and derive the full phase diagram in the low-energy subspace. Similar to the quantum dimer model and easy-axis kagome antiferromagnetic model studied before, we find an extended region of a gapped $\mathbb{Z}_2$ liquid with vison excitations. The gauge fluctuations, responsible for the vison modes, are dictated by the action of an *even* Ising gauge theory. In the ordered phase, where the vison gap closes, we observe a 3-fold rotationally symmetric loop ordering and present the critical theory for the amplitude fluctuations of the condensed modes. We also speculate the phase diagram for the fermionic counterpart of the model at all the above mentioned fractional fillings.

TT 6: Superconductivity: Cryodetectors

Time: Monday 9:30–12:30 Location: H 2053

TT 6.1 Mon 9:30 H 2053

Solid State Physics and Engineering to Push the Resolving Power of Magnetic Calorimeters Beyond 10 000 — •D. Hengstler, J. Geist, M. Keller, M. Krantz, C. Schötz, S. Kempf, L. Gastaldo, A. Fleischmann, and C. Enss — Kirchoff-Institute for Physics, Heidelberg University

Metallic magnetic calorimeters are energy dispersive particle detectors operated at temperatures below 100 mK. They make use of a paramagnetic temperature sensor to convert the energy that is deposited by an absorbed particle into a magnetic flux change in a SQUID, which can be read-out as a voltage signal with low noise and large bandwidth.

During the last decade we have been optimizing the signal size of MMCs by numerical optimizations and by the consequent use of microfabrication techniques, while lowering the readout noise close to quantum limit. The combination of both rewarded us recently with an instrumental linewidth of 1.6 eV (FWHM) for 6 keV x-rays, which is a world record. Operating this detector with optimal parameters the signal-to-noise-ratio is actually equivalent to an energy resolution below 1.0 eV (FWHM). At energies in the keV-range however, this resolution could not be achieved. Such discrepancies can arise from a-thermal phonon loss or position dependencies.

In this talk we summerize the physics of MMCs focusing on solid state effects and show recent results of these detectors in various applications. This includes the use of Ag:Er as a paramagnetic sensor material instead of Au:Er to increase the energy resolution at temperatures below 50 mK.

TT 6.2 Mon 9:45 H 2053

Investigation of low-frequency excess noise in low-T_c dc-SQUIDs — •Sebastian Kempf, Anna Ferring, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Germany.

Dc-SQUIDs are the most sensitive wideband devices for measuring physical quantities that can be naturally converted into magnetic flux. They show exceptional low noise over the full frequency range and are therefore heavily used in a variety of applications. However, they exhibit a low-frequency noise contribution with a spectral density scaling as $1/f^\alpha$ arising either from critical current fluctuations or magnetic flux noise, e.g. due to surface magnetic moments. While the first seems theoretically well understood, the origin of excess magnetic flux noise is still unknown.

Very recently, we have fabricated a set of single SQUIDs as well as N-SQUID series arrays, both employing Nb/Al-AlO_x/Nb Josephson junctions, and measured their noise spectra down to mK temperatures. We found that the magnitudes of the $1/f^\alpha$ noise expressed as energy sensitivities $\epsilon_{1/f}(1\,\mathrm{Hz})$ are as low as $34\,h$ at mK temperatures and that they increase with α. While $\alpha \leq 0.7$ for our single SQUIDs, our SQUID arrays show typically true $1/f$ noise with $\alpha \simeq 1$. We discuss our current data set in the context of present theories and compare it with data reported earlier. We also discuss an experimental method allowing for a direct measurement of noise spectra of single SQUIDs without the need of subtracting preamplifier noise and show first experimental results obtained with this method.

TT 6.3 Mon 10:00 H 2053

Large-area detectors for position and energy resolving detection of neutral molecular fragments at CSR — •L. Gamer[1], D. Schulz[1], A. Fleischmann[1], L. Gastaldo[1], S. Kempf[1], C. Krantz[2], O. Novotny[3], A. Wolf[2], and C. Enss[1] — [1]Heidelberg Univ. — [2]MPI-K Heidelberg — [3]Columbia Astrophysics Laboratory

We present a detector with a circular detection area of 10 cm^2 based on metallic magnetic calorimeters that is suited for position and energy sensitive measurements of neutral particle hits from fragmentation of molecular ion beams at the Cryogenic Storage Ring at MPI-K. It consists of 16 large area particle absorbers, arranged like the 16 slices of a pizza of radius 36 mm, where the temperature of each is monitored by a paramagnetic temperature sensor positioned along the outer absorber edges. Due to the finite thermal diffusivity in the absorbers, the signal rise-time is a measure of the radial event position while the integrated signal amplitude is proportional to the particle energy. We show very successful prove-of-principle experiments of this detector using x-ray photons. We discuss measurements where fragments of 150 keV molecules where stopped in massive gold absorbers showing that the production of lattice defects can cause a major contribution to linewidth in this energy and mass range. As an outlook we move on to a 4096 pixels detector covering a detection area of 20 cm^2. It consists of 1024 temperature sensors that are read out by only 32 SQUID channels. Each temperature sensor is coupled to 4 absorbers using different thermal links, thus allowing to locate the event position within a set of absorbers again by measuring the rise-time of the detector signal.

TT 6.4 Mon 10:15 H 2053

Feasibility Study for the Determination of Z-distributions of fission fragments with Calorimetric Low Temperature Detectors — •Patrick Grabitz[1,2], Peter Egelhof[1,2], Saskia Kraft-Bermuth[3], Pascal Scholz[3], Artur Echler[3], Shawn Bishop[4], Jose Gomez[4], Manfred Mutterer[1], and Victor Andrianov[1,3] — [1]GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany — [2]Universät Mainz, Germany — [3]Universität Gießen, Germany — [4]Technische Universität München

Compared to conventional ionization detectors calorimetric low temperature detectors (CLTD's) provide, due to their detection principle, substantial advantages in detector performance, such as energy resolution, linearity and the absence of any pulse height defect. One potential application of such detectors is the determination of nuclear charge distributions of fission fragments from thermal neutron induced fission at the LOHENGRIN mass separator (ILL, Grenoble) by using the absorber method. After passing the mass separator, fission fragments have the same mass and the same kinetic energy, but different nuclear charges. For the separation of the nuclear charges one can exploit their nuclear charge dependent energy loss after passing through an absorber foil. This separation requires a high energy resolution detector system as well as degrader foils, optimized with respect to thickness, homogeneity, etc. A test experiment performed at the tandem accelerator at Munich (MLL, LMU) with stable ^{109}Ag and ^{127}I beams with different kinetic energies has demonstrated a good Z-selectivity, and thus the feasibility of the experimental method.

TT 6.5 Mon 10:30 H 2053

SQUID-based noise thermometer for sub-Millikelvin refrigerators — •Marco Schmidt[1], Jörn Beyer[1], Monique Klemm[1], Sassan Alivaliollahi[2], and Henry Barthelmess[2] — [1]Physikalisch-Technische Bundesanstalt, Abbestraße 2-12, 10587 Berlin — [2]Magnicon GmbH, Barkhausenweg 11, 22339 Hamburg

The magnetic field fluctuation thermometer (MFFT) is a high-accuracy SQUID-based noise thermometer suitable for sub-Kelvin thermometry. A highly sensitive low-Tc SQUID magnetometer detects inductively the magnetic field fluctuation above a metal surface. The fluctuations are generated by the thermal activated noise currents inside the metal body that is thermally anchored to the temperature stage to be measured. The spectral shape is independent of temperature as the electrical conductivity is constant and the geometry is fixed. The magnetic noise power spectral amplitudes at any frequencies are directly proportional to temperature. Hence, only one reference measurement at a known temperature is required for calibration. A complete MFFT thermometer system for the temperature range of ca. 4 K down to <10 mK is commercially available. We have now developed an integrated MFFT with an extended range of operation down to <1 mK. For this purpose the sensitivity of the SQUID sensor has been increased, the metal body geometry modified and the magnetic shielding of the MFFT module improved. These modifications make it possible to obtain a thermometer noise temperature of <10 μK. We discuss the rationale for our MFFT configuration and present numerical simulations and experimental results.

TT 6.6 Mon 10:45 H 2053

Nanofabrication of coulomb blockade thermometers — •Matthias Meschke[1], Ossi M Hahtela[2], Anna V Feshchenko[1], Antti Kemppinen[2], Martti Heinonen[2], Antti Manninen[2], and Jukka P Pekola[1] — [1]Aalto University, Espoo, Finland — [2]Centre for Metrology and Accreditation (MIKES), Espoo, Finland

Coulomb blockade thermometry (CBT) is one example of a practical primary thermometer that relates temperature directly to Boltzmann's constant (kB) via a voltage measurement. Such primary methods are

required for the realization of a proposed new international temperature scale that relates to thermodynamic temperature via an exact definition of kB.

Using cutting-edge electron beam lithography, we demonstrate the fabrication of arrays of small enough structures (30 nm x 30 nm) combined with extreme homogeneity (5%) widening the useful temperature range of precise CBT to higher temperatures up to about 40 K. We present a characterization of the remaining fabrication inhomogeneities as a part of the uncertainty budget of CBT that is one prerequisite for CBT measurements satisfying metrological standards. An improved accuracy of CBT sensors at elevated temperatures directly enhances the performance at lower temperatures via the improved homogeneity and the possibility to operate CBT in a stronger CB regime with enhanced signal magnitude.

Finally, we describe an experimental comparison of CBT, consisting of arrays of many (about 1000) tunnel junctions to thermometry realized using only a single tunnel junction.

15 min. break.

TT 6.7 Mon 11:15 H 2053

Characterisation of micro and nano SQUIDs at variable temperature and magnetic field — •Claudia Köhn, Jan-Hendrik Storm, Sylke Bechstein, and Thomas Schurig — Physikalisch-Technische Bundesanstalt, Abbestraße 2-12, 10587 Berlin

SQUIDs are highly suited to investigate the magnetic properties of samples with small dimensions, such as nanoparticles, or to read out nanoelectromechanical systems (NEMS). Due to the small sample size, SQUIDs with dimensions in the μm or nm regime are desirable. These micro or nano SQUIDs should have a low noise and no hysteresis in the current-voltage-characteristic, even when operated in high magnetic fields of up to several 100 mT. To investigate such SQUID, we developed measurement setups which can simulate the measurement conditions of the intended SQUID application. The design and performance of two measurement setups will be shown and compared. One setup uses a dipstick that is immersed in liquid helium and can be evacuated to provide SQUID temperatures between 4.5 K and 10 K. The other one uses an evaporation cryostat so that the temperature can be varied from 2 K to 60 K. Both setups are equipped with coils to enable SQUID operation in variable magnetic field. To minimize noise, the output of the SQUID under test is preamplified by a SQUID series array which is operated at 4.2 K. First results of the characterisation of micro and nano SQUIDs will be presented.

This work was partly supported by the DFG under Grant No. SCHU1950/5-1 and within the European Metrology Research Program EMRP.

TT 6.8 Mon 11:30 H 2053

YBCO nanoSQUIDs applied to the investigation of small spin systems — •Maria Jose Martinez Perez[1], Tobias Schwarz[1], Roman Wölbing[1], Benedikt Müller[1], Christopher F. Reiche[2], Thomas Mühl[2], Bernd Büchner[2], Javier Sese[3], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut and Center for Collective Quantum Phenomena in LISA$^+$, Universität Tübingen, Germany — [2]Leibniz Institute for Solid State and Materials Research IFW Dresden, Germany — [3]Instituto de Nanociencia de Aragón and Advanced Microscopy Laboratory, Zaragoza, Spain

We present the realization of ultra-sensitive YBCO nanoSQUIDs based on submicron grain boundary junctions patterned by focused ion beam milling. White flux noise down to $\sim 50 n\Phi_0/Hz^{1/2}$ has been achieved, yielding spin sensitivities of down to a few $\mu_B/Hz^{1/2}$ at $T = 4.2$ K. Moreover, we demonstrate that magnetic fields up to the tesla range can be applied, fulfilling a fundamental condition for the study of small spin systems. As a proof-of-principle we present the successful deposition of a Fe-filled carbon nanotube (~ 40 nm in diameter and ~ 14 μm in length) and an individual Co nanopillar (base diameter of ~ 50 nm and height ~ 10 nm) close to the nanoSQUID loop. We show that submicrometric control over the particle position lead to large magnetic coupling factors between the nano-loop and the spin system. Together with the possibility of applying large magnetic fields, the latter has allowed us to directly observe the magnetization reversal of these spin systems at different temperatures.

TT 6.9 Mon 11:45 H 2053

Development of a Compact Low-Noise Pulse Tube Cryocooler for Operation of Superconducting Optical Detectors near 5 K — •Bernd Schmidt[1,2], Jens Falter[1], André Schirmeisen[1,2], and Günter Thummes[1,2] — [1]TransMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany — [2]Institute of Applied Physics (IAP), Justus-Liebig-University Giessen, Germany

The advantage of pulse tube cryocoolers (PTCs), when compared to Stirling- and Gifford-McMahon-coolers, is the absence of a cold moving displacer. This unique feature leads to a low level of mechanical vibrations, lower EMI, and increased reliability of the cold head. Therefore, two-stage PTCs are becoming more and more attractive for cryogen-free cooling at liquid-helium temperatures. The trend in the development of PTCs is towards high cooling powers, which reach up to more than 1 W at 4.2 K. However, the operation of many cryoelectronic devices requires only cooling powers well below 100 mW near 4-5 K. To date, the smallest 4 K PTC on the market operates with a 2 kW helium-compressor and delivers a cooling power of 250 mW at 4.2 K (TransMIT GmbH, model PTD4200). Within the new BMBF joint project "SUSY", we started the development of an even smaller two-stage PTC for cooling of superconducting IR-detectors at temperatures near 5 K. The compressor input power of this new cooler will be approx. 1 kW, significantly reducing the intrinsic residual vibrations of the cold head that result from the pressure-induced "breathing". The lower pressure oscillation will also improve the temperature stability. Work supported by the German BMBF under grant no. 13N13444

TT 6.10 Mon 12:00 H 2053

CFD-Simulations of a 4π-contiuous-mode dilution refrigerator for the CB-ELSA experiment — Timo Altfelde, Marcel Bornstein, Hartmut Dutz, Stefan Goertz, Roland Miebach, Scott Reeve, •Stefan Runkel, Marco Sommer, and Benjamin Streit — Physikalisches Institut, Bonn, Germany

The polarized target group at Bonn operates a dilution refrigerator for double polarization experiments at the Crystal Barrel in Bonn. To get high target polarizations and long relaxation times low temperatures are indispensable. To reach temperatures below 30 mK and to allow for the use of an internal polarization magnet, the polarized target group is building a new continuous mode dilution refrigerator. As a optimizing tool for the construction of dilution refrigerators and for a better understanding of the different incoming and outgoing fluid streams several CFD-simulations are done. First the different streams are simulated independently for different parts of the refrigerator to get a better estimation of the flow parameters. Then the simulation is extended to include the heat exchange between the different streams at the heat exchangers for different operational parameters of the refrigerator. Afterwards the precooling stages of the refrigerator will be tested to compare the predicted and the measured operational parameters.

TT 6.11 Mon 12:15 H 2053

Development of an thin, internal superconducting polarisation magnet for the Polarised Target — Timo Altfelde, •Marcel Bornstein, Hartmut Dutz, Stefan Goertz, Roland Miebach, Scott Reeve, Stefan Runkel, Marco Sommer, and Benjamin Streit — Physikalisches Institut, Bonn, Germany

In order to improve the figure of merit of double-polarisation experiments at CB-ELSA in Bonn, the Polarised Target is working on a new dilution refrigerator. For maximum polarisation of nucleons low temperatures and a high homogeneous magnetic field within the target area is needed. A thin, superconducting magnet is in development, which will create a continuous longitudinal magnetic field of 2.5 T and which will be used within the new refrigerator. The solenoidal geometry of this magnet uses two additional correction coils, placed at a well defined calculated position, for reaching the homogeneity criteria of 10^{-4} needed for the dynamic nuclear polarisation process. Practically, the superconducting wires as well as the correction coils have to be placed with maximum precision: Small fluctuations of the distance between the current loops can diminish the requested homogeneity.

TT 7: Transport: Quantum Coherence and Quantum Information Systems – Theory (jointly with HL, MA)

Time: Monday 9:30–13:00 Location: H 3005

TT 7.1 Mon 9:30 H 3005

Collective modes in the fluxonium qubit — •Gianluigi Catelani[1] and Giovanni Viola[2] — [1]Forschungszentrum Jülich, PGI-2 — [2]RWTH Aachen, IQI

In the fluxonium qubit, an array comprising a large number of identical Josephson junctions form a so-called superinductance. The superinductance is connected to a junction – the phase slip element – with a smaller Josephson energy and a different charging energy. We investigate the effects of unavoidable capacitive couplings to ground as well as non-linearities of the superinductance: they both introduce interactions between the low-energy qubit degree of freedom and higher-energy collective modes of the circuit. We also consider the role of the additional capacitances that are used to couple the qubit to a resonator for driving and read-out. We show that the interactions with the collective modes can affect not only the spectrum of the qubit but also its coherence.

Work supported in part by the EU under REA grant agreement CIG-618258

TT 7.2 Mon 9:45 H 3005

Optimal Control of Quantum Measurement — Daniel Egger and •Frank Wilhelm — Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

Pulses to steer the time evolution of quantum systems can be designed with optimal control theory. In most cases it is the coherent processes that can be controlled and one optimizes the time evolution towards a target unitary process, sometimes also in the presence of non-controllable incoherent processes. Here we show how to extend the GRAPE algorithm in the case where the incoherent processes are controllable and the target time evolution is a non-unitary quantum channel. We perform a gradient search on a fidelity measure based on Choi matrices. We illustrate our algorithm by optimizing a measurement pulse for superconducting phase qubits. We show how this technique can lead to large measurement contrast close to 99%. We also show, within the validity of our model, that this algorithm can produce short 1.4 ns pulses with 98.2% contrast.

TT 7.3 Mon 10:00 H 3005

Optimal control of single flux quantum pulses — •Per Liebermann, Daniel Egger, and Frank Wilhelm — Universität des Saarlandes, Saarbrücken

Rapid single flux quantum pulses are a natural candidate for on-chip control of superconducting qubits [1]. We apply trains of single flux quantum pulses to perform single qubit gates. Under the constraint of constant amplitudes and gate times we use genetic algorithms for optimising the pulse sequence to decrease the gate error by two orders of magnitude. We consider leakage transitions into a third energy level as well as timing jitter of the pulses, exploring the robustness of our optimized sequence. This takes us one step further to on-chip qubit controls.

[1] R. McDermott and M.G. Vavilov, Phys. Rev. Applied 2, 014007 (2014)

TT 7.4 Mon 10:15 H 3005

Adaptive characterization of coherent states — •Markku P. V. Stenberg, Kevin Pack, and Frank K. Wilhelm — Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

We present a method for efficient characterization of an optical coherent state $|\alpha\rangle$. We choose measurement setups adaptively based on the data while it is collected. Our algorithm divides the estimation in three different steps with different measurement strategies: (i) searching a crude estimate, (ii) rapidly improving the accuracy, and (iii) the phase where the improvement of the accuracy slows down due to the quantum nature of the coherent state. Our algorithm significantly outperforms nonadaptive schemes. While our standard strategy is robust against measurement errors we also present strategies optimized for the presence of such errors.

TT 7.5 Mon 10:30 H 3005

Qubit dephasing due to Quasiparticle Tunneling — •Sebastian Zanker, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany

We study dephasing of a superconducting qubit due to quasiparticle tunneling through a Josephson junction. While qubit decay due to tunneling processes is well understood within a golden rule approximation, pure dephasing due to BCS quasiparticles gives rise to a divergent golden rule rate. We calculate qubit dephasing due to quasiparticle tunneling beyond lowest order approximation in coupling between qubit and quasiparticles. Summing up a certain class of diagrams we show that qubit dephasing due to purely longitudinal coupling to quasiparticles leads to dephasing $\sim \exp(-x(t))$ where $x(t) \propto t^{3/2}$ for short time scales and $x(t) \propto t \log(t)$ for long time scales.

TT 7.6 Mon 10:45 H 3005

Detecting nonlocal Cooper pair entanglement by optical Bell inequality violation — Simon E. Nigg, Rakesh P. Tiwari, Stefan Walter, and •Thomas L. Schmidt — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

Based on the Bardeen Cooper Schrieffer (BCS) theory of superconductivity, the coherent splitting of Cooper pairs from a superconductor to two spatially separated quantum dots has been predicted to generate nonlocal pairs of entangled electrons. In order to test this hypothesis, we propose a scheme to transfer the spin state of a split Cooper pair onto the polarization state of a pair of optical photons. We show that the produced photon pairs can be used to violate a Bell inequality, unambiguously demonstrating the entanglement of the split Cooper pairs.

[1] Nigg et al., arXiv:1411.3945 [cond-mat.mes-hall]

TT 7.7 Mon 11:00 H 3005

Detection of non-local spin-entanglement by light emission from a superconducting pn-junction — •Alexander Schroer and Patrik Recher — Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig, Germany

We model a superconducting pn-junction in which the n- and the p-site are contacted through two optical quantum dots, each embedded into a photonic nanocavity. Whenever a Cooper pair is transported from the n-site to the p-site, two photons are emitted. When the two electrons of a Cooper pair are transported through different quantum dots, polarization entangled photons are created, provided that the Cooper pairs retain their spin-singlet character although being spatially separated on the two quantum dots. We show that a CHSH Bell-type measurement is able to detect the entanglement of the photons over a broad range of microscopic parameters, even in the presence of parasitic processes and imperfections. Observing this signature is a direct proof of crossed Andreev reflection, or, equivalently, Cooper pair splitting, retaining the spin-singlet wave function.

15 min. break.

TT 7.8 Mon 11:30 H 3005

Scattering of two photons from two distant qubits: exact solution — Matti Laakso and •Mikhail Pletyukhov — Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen

We consider the inelastic scattering of two photons from two qubits separated by an arbitrary distance and coupled to a one-dimensional transmission line. We present an exact, analytical solution to the problem, and use it to explore a particular configuration of qubits which is transparent to single-photon scattering, thus highlighting non-Markovian effects of inelastic two-photon scattering: Strong two-photon interference and momentum dependent photon (anti)bunching. This latter effect can be seen as an inelastic generalization of the Hong-Ou-Mandel effect.

TT 7.9 Mon 11:45 H 3005

Robust entanglement under multipartite correlated dephasing — •Edoardo Carnio[1,2], Manuel Gessner[2], and Andreas Buchleitner[2,3] — [1]Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom — [2]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3,

79104 Freiburg, Germany — [3]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität Freiburg, Albertstraße 19, 79104 Freiburg, Germany

We derive an analytical description for the dephasing process undergone by a system on non-interacting atomic qubits, immersed in a uniform, fluctuating magnetic field. The dephasing process is correlated, as the noise source is common to all the particles and induces an effective atom-atom interaction on them. This correlated nature allows to specify field orientations that preserve any degree of atomic entanglement for all times, and families of states with entanglement properties that are time-invariant for arbitrary field orientations. Our formalism applies to arbitrary spectral distributions of the fluctuations.

TT 7.10 Mon 12:00 H 3005

Bell inequalities and waiting times — •Christina Pöltl and Michele Governale — School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, PO Box 600, Wellington 6140, New Zealand

We propose a Bell test based on waiting time distributions for spin entangled electron pairs, which are generated and split in mesoscopic Coulomb blockade structures, denoted as entanglers. These systems have the advantage that quantum point contacts enable a time resolved observation of the electrons occupying the system, which gives access to quantities such as full counting statistics and waiting time distributions. We use the partial waiting times to define a CHSH-Bell test, which is a purely electronic analogue of the test used in quantum optics. After the introduction of the Bell inequality we discuss the findings on the two examples of a double quantum dot and a triple quantum dot. This Bell test allows the exclusion of irrelevant tunnel processes from the statistics normally used for the Bell correlations. This can improve the parameter range for which a violation of the Bell inequality can be measured significantly.

TT 7.11 Mon 12:15 H 3005

Quantum dynamics of a strongly driven Josephson Junction — •Jennifer Gosner, Björn Kubala, and Joachim Ankerhold — Institute for Complex Quantum Systems, University of Ulm, Germany

A Josephson Junction embedded in a dissipative circuit can be driven to exhibit non-linear oscillations.

Classically the non-linear oscillator shows under sufficient strong driving and weak damping dynamical bifurcations and a bistable region similar to the conventional Duffing-oscillator. These features depend sensitively on initial conditions and parameters. The sensitivity of this circuit, called Josephson Bifurcation Amplifier, can be used to amplify an incoming signal, to form a sensing device or even for measuring a quantum system.

The *quantum* dynamics can be described by a dissipative Lindblad master equation. Signatures of the classical bifurcation phenomena appear in the Wigner representation, used to characterize and visualize the resulting behaviour. In order to compare this quantum dynamics to that of the conventional Duffing-oscillator, the complete cosine-nonlinearity of the Josephson Junction is kept for the quantum description while going into a rotating frame.

TT 7.12 Mon 12:30 H 3005

Dissipation-induced first order decoherence phase transition in a non-interacting fermionic system — •Mihailo Cubrovic — Institute for Theoretical Physics, Universität zu Köln, Zülpicher Str. 77, D-50937, Köln, Germany

We consider a dissipative tight-binding fermionic chain as a model for a nanowire with current leakage due to imperfect isolation. The dissipation manifests as tunneling into/out of the chain from/to the environment. The evolution of the system is described by the Lindblad equation, generalized to incorporate the memory effects in the bath. Already infinitesimally small dissipation along the chain induces a quantum phase transition (QPT). This is a decoherence QPT: the reduced density matrix of a subsystem (far from the ends of the chain) can be represented as the tensor product of single-site density matrices. We analyze the QPT in the thermodynamic limit by looking at the entropy and the response function in the bulk, and compare in detail the results with and without memory in the bath. To gain a better intuitive understanding we also contruct the analogous classical model (a correlated random walk process) and compare its behavior to the QPT of the quantum chain.

TT 7.13 Mon 12:45 H 3005

Spin dynamics using the Majorana representation: validity, path integral and higher correlators — •Pablo Schad[1], Boris N. Narozhny[1,2], Gerd Schön[3], Yuriy Makhlin[4,5], and Alexander Shnirman[1] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [2]National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe shosse 31, 115409 Moscow, Russia — [3]Institut für Theoretische Festkörperphysik und Institut für Nanotechnologie, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [4]Landau Institute for Theoretical Physics, acad. Semyonov av., 1a, 142432, Chernogolovka, Russia — [5]Moscow Institute of Physics and Technology, 141700, Dolgoprudny, Russia

We present a method to calculate higher spin correlators via the Majorana fermion representation of spin operators. We show explicitly that the Majorana representation does not require any projection procedure. Previously found identities [1,2] between spin and Majorana fermion correlation functions are extended. As an example we consider a spin-1/2 coupled to an isotropic, ohmic bath. We formulate a path-integral approach, which is valid at B=0 in contrast to perturbation theory, find the saddle-point solution and discuss fluctuations. We demonstrate that spin correlators in the high-temperature regime can be obtained using saddle-point Green's functions.

[1] A. Shnirman and Y. Makhlin,
Phys. Rev. Lett. 91, 207204 (2003).
[2] W. Mao, P. Coleman, C. Hooley, and D. Langreth,
Phys. Rev. Lett. 91, 207203 (2003).

TT 8: Low-Dimensional Systems: Oxide Hetero-Interfaces

Time: Monday 9:30–12:30 Location: H 3010

TT 8.1 Mon 9:30 H 3010

Transport properties of $LaAlO_3/SrTiO_3$ nanostructures — •Alexander Müller[1], Mohsin Minhas[1], Hans-Helmuth Blaschek[1], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale) , Germany

Deposition of thin layers of $LaAlO_3$ (LAO) on top of a TiO_2 terminated $SrTiO_3$ (STO) substrate with Pulsed Laser Deposition results in a two dimensional electron gas at the interface [1]. Using PMMA as resist and etch mask this electron gas can be patterned by a standard electron-beam lithography step and subsequent Reactive Ion Etching to remove the LAO.

With this process transport structures with minimum dimensions in the sub-micron regime have been fabricated. The structures include gaps of approx. 100 nm width. Transport through the gap is characterized by taking I/V characteristics in a standard four point geometry from room temperature down to 1.5 K.

Between 1.5 and 30 K up to a threshold voltage of tens of mV no current is observed. Beyond that threshold voltage the current increases dramatically. Within a few tens of mV the current can increase by up to eight orders of magnitude. The threshold voltage is temperature dependent in a non-monotonic fashion and all I/V curves are free of any hysteresis.

[1] A. Ohtomo, H.Y. Hwang, Nature **427**, 6973 (2004)

TT 8.2 Mon 9:45 H 3010

An industry compatible low-damage nano-patterning process for LAO/STO heterostructures — •Mohsin Zamir Minhas[1], Hans-Helmuth Blaschek[1], Frank Heyroth[2], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle (Saale) , Germany

The discovery of an electron gas at the interface between the two band

insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO)[1] has initiated a huge effort to study this interface in detail. Later on other interesting properties such as induced ferromagnetism[2] and superconductivity[3] have been reported which make the LAO/STO interface a model system to study the fundamental physics of strongly correlated electronic system and also a candidate for future multifunctional oxide electronics. A reproducible nano-patterning technique is required to develop this unique interface into useful technologies. Here we present a reliable technique to physically pattern the quasi-two-dimensional electron gas (q2DEG) down to lateral dimensions as small as 100nm while maintaining its conducting properties. The fully industry compatible process uses electron beam lithography in combination with reactive ion etching. Temperature dependent transport properties of patterned Hall bars of various widths show a small size dependence of conductivity. The deviation can be explained by a narrow lateral depletion region.

[1] Ohtomo, A. et al. Nature 427 (2004) 423.
[2] Brinkman, A. et al. Nat. Mater. 6 (2007) 493.
[3] Reyren, N. et al. Science 317 (2007) 1196.

TT 8.3 Mon 10:00 H 3010

Valence Band Electronic Structure and Band Alignment of $LaAlO_3/SrTiO_3$(111) Heterointerfaces — •J. Gabel[1], P. Scheiderer[1], M. Zapf[1], P. Schütz[1], C. Schlüter[2], T.-L. Lee[2], M. Sing[1], and R. Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg — [2]Diamond Light Source, Didcot

As in the famous $LaAlO_3$(LAO)/$SrTiO_3$(STO) (001) a two-dimensional electron system (2DES) also forms at the interface between LAO and STO in (111) orientation. A distinct feature of the (111) interface is its peculiar real space topology. Each bilayer represents a buckled honeycomb lattice similar to graphene which is known theoretically to host various topologically non-trivial states. Bilayer STO in proximity to the interface can be regarded as a three-orbital generalization of graphene with enhanced electron correlations making it a promising candidate for the realization of strongly correlated topological phases. We have investigated the electronic structure of the LAO/STO (111) heterostructure in relation to the oxygen vacancy concentration which we can control by synchrotron light irradiation and oxygen dosing. With hard X-ray photoemission we study the core levels, whereas resonant soft X-ray photoemission is used to probe the interfacial valence band (VB) states. Two VB features are found: a peak at the Fermi level associated with the 2DES and in-gap states at higher binding energies attributed to oxygen vacancies. By varying the oxygen vacancy contribution we can tune the emergence of the VB states and engineer the interfacial band alignment.

TT 8.4 Mon 10:15 H 3010

Oxygen Dosing the Surface of $SrTiO_3$ — •L. Dudy[1], P. Scheiderer[1], J.D. Denlinger[2], P. Schütz[1], J. Gabel[1], M. Buchwald[1], C. Schlueter[3], T.-L. Lee[3], M. Sing[1], and R. Claessen[1] — [1]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, 94270, USA — [3]Diamond Light Source Ltd., Didcot, Oxfordshire OX11 0DE, United Kingdom

The highly mobile two-dimensional electron system (2DES) on the surface of the insulating $SrTiO_3$(STO) offers exciting perspectives for advanced material design. This 2DES resides in a depletion layer caused by oxygen deficiency of the surface. With photoemission spectroscopy, we monitor the appearance of quasi-particle weight (QP) at the Fermi energy and oxygen vacancy induced states in the band gap (IG). Both, QP and IG weight, increase and decrease respectively upon exposure to extreme ultraviolet (XUV) light and in-situ oxygen dosing. By a proper adjustment of oxygen dosing, any intermediate state can be stabilized providing full control over the charge carrier density. From a comparison of the charge carrier concentrations obtained from an analysis of core-level spectra and the Fermi-surface volume, we conclude on a spatially inhomogeneous surface electronic structure with at least two different phases.

TT 8.5 Mon 10:30 H 3010

***Ab initio* determination of the spin texture in $SrTiO_3$ surfaces** — •Michaela Altmeyer[1], Klaus Koepernik[2], Harald O. Jeschke[1], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]IFW, 01171 Dresden, Germany

The appearance of oxygen vacancies in a surface of strontium titanate has been recently identified to be a likely reason for the formation of a two-dimensional electron gas close to the surface. Lately the first SARPES measurements [1] on these surfaces unveiled an interesting spin texture which shows besides the expected Rashba effect a huge spin splitting that can not be attributed to spin-orbit interaction. Employing density functional theory we therefore examined oxygen deficient slabs and found that indeed magnetism is capable of explaining the measured spin splittings. Moreover we obtain a very rich spin texture where we find not only rotating spins due to the Rashba interaction, but a very complex spin structure most likely caused by an interplay of orbital and spin degrees of freedom.

[1] A.F. Santander-Syro *et al.*, Nature Materials **13**, 1085 (2014).

TT 8.6 Mon 10:45 H 3010

Effect of band filling and symmetry breaking on the electronic ground state in $(LaXO_3)_2/(LaAlO_3)_4$(111) (X = 3d) superlattices — •David Doennig[1], Warren E. Pickett[2], and Rossitza Pentcheva[3,1] — [1]Forschungs-Neutronenquelle (FRMII), TU München — [2]University of California Davis, U.S.A. — [3]Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Structural patterns, e.g. a buckled honeycomb lattice, realized in (111)-oriented perovskite bilayers may lead to exotic electronic ground states such as a Dirac-point Fermi surface [1-3]. Based on density functional theory calculations including a Hubbard U term, we explore systematically the effect of band filling in [111]-oriented $(LaXO_3)_2/(LaAlO_3)_4$ superlattices with X spanning the series of open shell 3d ions. The interplay of charge, spin, orbital, and lattice degrees of freedom reveals some regularities over the series, but also several unexpected symmetry lowering reconstructions that can guide the design of artificial materials with desired spin-charge-orbital order in conjunction with size of the energy gap and the possibility for emergent topological character. We acknowledge funding by the DFG (SFB/TR80, project G3).

[1] D. Xiao *et al.*, Nat. Commun. **2**, 596 (2011).
[2] D. Doennig, W. E. Pickett, and R. Pentcheva, Phys. Rev. Lett. **111**, 126804 (2013).
[3] D. Doennig, W. E. Pickett, and R. Pentcheva, Phys. Rev. B **89**, 121110(R) (2014).

15 min. break.

TT 8.7 Mon 11:15 H 3010

Towards Mott design by δ-doping of strongly correlated titanates — •Frank Lechermann and Michael Obermeyer — I. Institut für Theoretische Physik, Universität Hamburg

Oxide heterostructures are promising systems for exploring novel composite materials beyond nature's original conception. Already the doping of distorted-perovskite Mott-insulating titanates such as $LaTiO_3$ and $GdTiO_3$ with a single SrO layer gives rise to a rich correlated electronic structure [1]. A realistic superlattice study by means of the charge self-consistent combination of density functional theory (DFT) with dynamical mean-field theory (DMFT) reveals layer- and temperature-dependent multi-orbital metal-insulator transitions. Doped along the [001] direction, an orbital-selective metallic layer at the interface dissolves via an orbital-polarized doped-Mott state into an orbital-ordered insulating regime beyond the two conducting TiO_2 layers. Breaking the spin symmetry in δ-doped $GdTiO_3$ results in blocks of ferromagnetic itinerant and ferromagnetic Mott-insulating layers which are coupled antiferromagnetically.

[1] F. Lechermann and M. Obermeyer, arXiv:1411.1637 (2014)

TT 8.8 Mon 11:30 H 3010

DFT+DMFT study of strain and interface effects in $LaTiO_3$ and $LaVO_3$ — Krzysztof Dymkowski, Gabriele Sclauzero, and •Claude Ederer — Materials Theory, ETH Zurich, Switzerland

Metal-insulator transitions in thin films of early transition metal correlated oxides are linked to both epitaxial strain and electronic reconstruction at the film/substrate interface. We separately address these two key factors for $LaTiO_3$ and $LaVO_3$ through density functional theory plus dynamical mean-field theory (DFT+DMFT). We find that mere epitaxial strain suffices to induce an insulator-to-metal transition in $LaTiO_3$ [1], but not in $LaVO_3$, in agreement with recent experiments [2]. We show that this difference can be explained by the combined effect of strain-induced changes in the crystal field splitting of t_{2g} orbitals and different orbital filling in these two materials. The

role of the interface is investigated through DFT+DMFT simulations of $LaVO_3/SrTiO_3$ heterostructures with varying superlattice periodicities and substrate terminations. Our aim is to assess whether the metallicity observed at the LaVO3/SrTiO3 interface could be driven by pure electronic reconstruction effects, rather than structural or stoichiometric reasons (such as, e.g., O-related defects).

[1] Dymkowski/Ederer, Phys. Rev. B 89, 161109 (2014).
[2] He et al., Phys. Rev. B 86, 081401 (2012).

TT 8.9 Mon 11:45 H 3010

$LaAlO_3$–$LaNiO_3$ (111) interfaces: a DFT+DMFT study — •Oleg Janson and Karsten Held — Institut für Festkörperphysik, Technische Universität Wien, Österreich

As a peculiarity of (111) perovskite interfaces, the e_g electrons can retain their degeneracy and facilitate the emergence of topological phases. From the materials perspective, $LaAlO_3$–$LaNiO_3$ (111) interfaces based on Ni^{3+} are among the most promising candidates. A recent DFT+U study predicted a sizable orbital polarization for 1/1 (double perovskite) interfaces and a multiferroic behavior for Ni-bilayers [2]. Here, we further explore the properties of $LaAlO_3$-$LaNiO_3$ (111) interfaces by considering purely local as well as cooperative Jahn-Teller distortions and taking dynamical electronic correlations into account. Possible terminations and orbital reconstructions of these highly polar surfaces will be discussed. This work has been supported in part by European Research Council under the European Union's Seventh Framework Programme (FP/2007-2013)/ERC through grant agreement n. 306447.

[1] A. Rüegg and G. A. Fiete, Phys. Rev. B **84**, 201103 (2011).
[2] D. Doennig, W. E. Pickett and R. Pentcheva, Phys. Rev. B **89**, 121110 (2014).

TT 8.10 Mon 12:00 H 3010

Spin-orbit controlled capacitance of a polar heterostructure — •Kevin Steffen[1], Florian Loder[2], and Thilo Kopp[1] — [1]Center for Electronic Correlations and Magnetism, EP VI, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Center for Electronic Correlations and Magnetism, EP VI and TP III, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Oxide heterostructures with polar films display special electronic properties, such as the electronic reconstruction at their internal interfaces with the formation of two-dimensional metallic states. Moreover, the electrical field from the polar layers is inversion-symmetry breaking and may generate a strong Rashba spin-orbit coupling (RSOC) in the interfacial electronic system. We investigate the capacitance of a heterostructure in which a strong RSOC at a metallic interface is controlled by the electric field of a surface electrode. Such a structure is for example given by a $LaAlO_3$ film on a $SrTiO_3$ substrate which is gated by a top electrode. We find that due to a strong RSOC the capacitance can be larger than the classical geometric value.

TT 8.11 Mon 12:15 H 3010

Magnetism and Charge Transfer in $PrNiO_3$-$La_{0.7}Ca_{0.3}MnO_3$ Heterostructures — •Martin Bluschke[1,2], Alex Frano[1,2], Enrico Schierle[2], Matthias Hepting[1], Matteo Minola[1], Georg Christiani[1], Gennady Logvenov[1], Eugen Weschke[2], Eva Benckiser[1], and Bernhard Keimer[1] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Helmholz-Zentrum Berlin, Germany

Heterostructures of the bulk antiferromagnet $PrNiO_3$ (PNO) and the bulk ferromagnetic metal $La_{0.7}Ca_{0.3}MnO_3$ (LCMO) are grown by pulsed laser deposition on $LaSrAlO_4$ substrates for a systematic series of superlattice geometries. A characterization of the structural, magnetization, and transport properties is combined with the results of soft x-ray absorption and resonant scattering measurements to understand how the bulk properties of the individual components are modified via epitaxial strain and heterostructuring. In particular the PNO-LCMO interface is studied. A net transfer of electrons from Mn to Ni sites is observed near the interface. In addition the saturation magnetization and Curie temperature of the ferromagnetic response are found to be reduced compared to bulk LCMO. The antiferromagnetic order characteristic of bulk PNO is observed in superlattices containing 8 unit cells of PNO per bilayer, but suppressed below the detection limit for thinner 4 unit cell layers. Finally a transition between metallic and insulating behaviour in PNO is observed as the layer thickness is reduced from 12 to 4 unit cells, whereas the LCMO layers studied (4-18 unit cells) were insulating in all cases.

TT 9: Transport: Spintronics and Magnetotransport (jointly with HL, MA)

Time: Monday 9:30–12:00 Location: A 053

TT 9.1 Mon 9:30 A 053

Low Temperature THz Spectroscopy and Transport in Nanostructures — •Julian Braun, Sergej Andreev, Elke Scheer, and Torsten Pietsch — Universität Konstanz, Konstanz, Germany

Theoretical predictions [1] suggest a new source for THz radiation, based on a spin relaxation in metallic heterocontacts. In a dilute ferromagnet a spin imbalance can be created by a spin polarized current originating in a ferromagnet of opposite magnetization. Relaxation in the energetically more favorable spin distribution should occur by emission of a photon with an energy in the THz range.

We constructed a compact cw-THz spectrometer working at temperatures down to 4 K and a frequency range from 0.1 GHz to 2000 GHz. Installed in a vector magnet we can thereby correlate magnetotransport measurements with the spectroscopic analysis to investigate the spin imbalance in metallic heterocontacts. Additionally characterization measurement on different metallic and superconducting samples will be presented.

[1] A.M. Kadigrobov et al., Europhys. Lett. 67, 948-954 (2004).

TT 9.2 Mon 9:45 A 053

Room-Temperature Spin Thermoelectrics in Metallic Films — •Sebastian Tölle[1], Cosimo Gorini[2], and Ulrich Eckern[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Faculty of Physics, University of Regensburg, 93040 Regensburg, Germany

Efficient heat-to-spin conversion is the central goal of spin caloritronics. When considering metallic systems, two interesting phenomena stand out in this field: the spin Nernst effect and thermally-induced spin polarizations. They consist in the generation of, respectively, a spin current or a spin polarization transverse to an applied temperature gradient, i.e., they are the thermal counterparts of the well known spin Hall effect and current-induced spin polarization (Edelstein effect). We study these phenomena considering dynamical spin-orbit coupling, namely the spin-orbit coupling with phonons and vibrating impurities, which give rise to a dynamical side-jump mechanism and dynamical Elliott-Yafet spin relaxation. Such processes, which have not been considered before in this context, dominate at temperatures $T > T_D$, with T_D the Debye temperature. This condition is met in typical spin injection/extraction experiments performed at room temperature in transition metals such as Pt, Au, and Ta. Our results show a nonlinear T-dependence of the spin Nernst and spin Hall conductivities due to an interplay between intrinsic (Bychkov-Rashba type) and extrinsic (dynamical) spin-orbit coupling [1].

[1] S. Tölle, C. Gorini, and U. Eckern, arXiv:1409.1809 (2014) (accepted for publication in Phys. Rev. B).

TT 9.3 Mon 10:00 A 053

Phonon Skew Scattering — •Cosimo Gorini[1], Ulrich Eckern[2], and Roberto Raimondi[3] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Institut für Physik, Universität Augsburg — [3]Dipartimento di Fisica, Università Roma Tre

In spin injection/extraction experiments in metallic systems, the observed temperature behaviour of the (inverse) spin Hall effect is used to determine the dominant spin-orbit mechanism in the sample. This is a fundamental issue of high practical importance.

The current understanding of the high-T behaviour is based on a phenomenological extrapolation from the low-T theory. The latter predicts that (i) a T-independent (inverse) spin hall signal is a signature of dominant side-jump, and (ii) its scaling as the mobility indicates

dominant skew scattering.

Our quantum field theoretical (Keldysh) calculation shows, however, that at typical experimental temperatures phonon-induced skew scattering also leads to a T-independent signal – just as side-jump does. Thus, discerning between the two appears a more complicated issue than until now expected.

TT 9.4 Mon 10:15 A 053

Single atom memory described by the quantum master equation: Ho on Pt(111) — •Christian Karlewski[1,2], Michael Marthaler[1], Wulf Wulfhekel[3], and Gerd Schön[1,2] — [1]TFP, Karlsruher Institut für Technologie — [2]INT, Karlsruher Institut für Technologie — [3]PHI, Karlsruher Institut für Technologie

Miniaturizing current memory bits to optimize the storage density is an important task of information technology research. The ultimate goal are single atoms as one bit. Single magnetic holmium atoms on a platinum (111) surface have been investigated in Nature 503, 242 (2013) and have highly stable magnetic moments, in or out of the plane. Stability can be maintained for several minutes, making holmium a great candidate as single atomic storage. The theoretical description of this system is based on the quantum master equation of open quantum systems. We will show that even if the system in total behaves as a classical bit with two states, a full quantum mechanical description is needed to catch the dynamics properly. The dependence of the lifetime of this system on different parameters is investigated and we will show that it might be possible to improve the properties of our system even further by understanding the mechanisms which at present limit the lifetimes.

TT 9.5 Mon 10:30 A 053

Observation of spatial fluctuations of the Rashba parameter by scanning tunneling spectroscopy — •Jan Raphael Bindel[1], Marcus Liebmann[1], Jascha Ulrich[2], Eugene Sherman[3], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University, Aachen, Germany — [2]Institute for Quantum Information, RWTH Aachen University, Aachen, Germany — [3]Basque Foundation for Science, Ikerbasque, Bilbao, Spain

We investigate a 2DES induced by Cs surface doping of p-type InSb(110) and evaluate the Rashba parameter on the local scale. The Rashba effect is one of the possibilities to manipulate spins by external gate voltages which led to the proposal of the spin transistor. As a local property, however, the Rashba effect is prone to disorder as ubiquitous in semiconductors, which, in turn, induces spatial fluctuations of the strength of the Rashba effect, and, thus, spin dephasing [1]. Recently, we have shown that the Rashba effect can be probed by STS in magnetic fields as an additional contribution to the spin splitting [2]. Here, we investigate the correlations between the electrostatic potential and the Rashba effect on the local scale. A detailed magnetic field dependence analysis of the spin splitting is required in order to disentangle the Rashba parameter from the Zeeman effect and the spatially fluctuating exchange enhancement. Moreover the nodal structure of the wave functions has to be considered in higher Landau levels, where it leads to multiple peak structures [3].

[1] Glazov et al., Physica E 42, 2157 (2010).
[2] Becker et al., PRB 81, 155308 (2010).
[3] Hernangómez-Pérez et al., PRB 88, 245433 (2013).

15 min. break.

TT 9.6 Mon 11:00 A 053

Magnetoresistance in Weyl semimetals — •Janina Klier[1,2], Igor Gornyi[1,3], and Alexander Mirlin[1,2,4] — [1]Institute for Nanotechnology, Karlsruher Institute for Technology, Karlsruhe, Germany — [2]Institute for Theoretical Condensed Matter physics, Karlsruher Institute for Technology, Karlsruhe, Geermany — [3]A.F. Ioffe Physico-Technical Institute, St. Petersburg, Russia — [4]Petersburg Nuclear Physics Institute, St. Petersburg, Russia

We theoretically study the magnetoresistvity of a Weyl semimetal within two disorder models: pointlike impurities and charged impurities. Impurity scattering is treated using a self-consistent Born approximation. We find an unusual broadening of Landau levels which leads to a rich structure of various regimes in temperature-magnetic field plane. In particular, the magnetoresitance shows non-monotonous behavior. In the limits of strongest magnetic fields for pointlike impurities, this leads to a vanishing magnetoresistance. For charged impurities, broadening of Landau levels is less important in high magnetic fields. This leads to a positive linear magnetoresistance in strongest magnetic fields.

TT 9.7 Mon 11:15 A 053

Spin-orbit induced longitudinal spin transport in non-magnetic solids — •Sebastian Wimmer, Marten Seemann, Kristina Chadova, Diemo Ködderitzsch, and Hubert Ebert — Ludwig-Maximilians-Universität München, München, Deutschland

A group-theoretical scheme is presented that allows investigating the symmetry properties of response tensors relevant to the field of spintronics. For the spin conductivity tensor it is shown that only the magnetic Laue group has to be considered in this context. In this case non-vanishing transverse elements, found without making reference to the two-current model, give rise to the spin Hall and Edelstein effects in non-magnetic as well as magnetic solids. In the latter case non-vanishing longitudinal elements cause among others the spin-dependent Seebeck effect. For non-magnetic solids having low symmetry non-vanishing longitudinal elements are shown to exist as well. These give rise to spin-orbit induced *longitudinal* spin transport that has not been considered before. Numerical studies confirm these findings and demonstrate that the longitudinal spin conductivity may be in the same order of magnitude as the conventional transverse one.

TT 9.8 Mon 11:30 A 053

Topological transitions in the geometric phase in spin interferometers — •Henri Saarikoski[1], Enrique Vazquez[2], Jose Pablo Baltanás[2], Diego Frustaglia[2], Fumiya Nagasawa[3], and Junsaku Nitta[3] — [1]RIKEN Center for Emergent Matter Science (CEMS), Saitama 351-0198, Japan — [2]Departamento de Física Aplicada II, Universidad de Sevilla, E-41012 Sevilla, Spain — [3]Department of Materials Science, Tohoku University, Sendai 980-8579, Japan

An electronic spin transported around a circuit acquires a phase factor that depends on the geometry of the path in the parameter space. In the adiabatic limit this is the Berry phase and it has been argued that it can undergo an abrupt transition via manipulation of the topology of the path [1]. However, spin transport in mesoscopic structures is usually nonadiabatic, which is associated with the Aharonov-Anandan geometric phase. Here we identify the characteristic signatures of topological transitions in nonadiabatic spin transport by 1D and 2D calculations of mesoscopic loops. We find that the topological transition is characterized by an *effective* Berry phase due to correlations between dynamic and geometric phases close to the region where the transition occurs. This effective Berry phase is related to the topology of the field texture rather than the spin-state structure. The transition manifests as a distinct dislocation of the interference pattern in the quantum conductance. The phenomenon is robust, and can be observed in mesoscopic arrays of loops where phase coherence is significant.

[1] Y. Lyanda-Geller, Phys. Rev. Lett. 71, 657 (1993).

TT 9.9 Mon 11:45 A 053

Use of resonant tunneling in spin transfer torque magnetic tunnel junctions — •Bhaskaran Muralidharan[1], Niladri Chatterji[2], and Ashwin Tulapurkar[1] — [1]Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India — [2]Department of Physics, IIT Bombay, Powai, Mumbai- 400076, India

We propose a novel device that uses resonant tunneling to enhance the spin-transfer torque switching characteristics of magnetic tunnel junctions. The proposed device structure is a resonant tunneling magnetic tunnel junction based on a MgO-semiconductor heterostructure sandwiched between a fixed magnet and a free magnet [1]. We employ the non-equilibrium Green's function formalism coupled self consistently with the Landau-Lifshitz-Gilbert-Slonczewski equation to demonstrate that the physics of resonant tunneling leads to improved tunnel magneto-resistance characteristics as well as lower switching voltages in comparison with traditional trilayer devices. Using this framework, we also demonstrate a novel spin torque oscillator design at zero applied magnetic field, by simply engineering parallel and perpendicular spin torques.

[1] N. Chatterji, A. A. Tulapurkar and B. Muralidharan, ArXiv: 1411.6454, (2014).

TT 10: Organic Electronics and Photovoltaics (organized by DS)

Time: Monday 9:30–13:00 Location: H 2032

TT 10.1 Mon 9:30 H 2032

Metal-organic interfaces: from molecular self-assembly to electronic transport through ultrathin functional monolayers — •Florian von Wrochem — Sony Deutschland GmbH, Stuttgart

The continuous development of organic electronic devices, combined with the advances in spectroscopy and electrical characterization, dramatically extended our understanding of the physical and chemical processes occurring at metal/organic interfaces. Here, an overview of experimental and theoretical efforts aiming towards the selective modification of interfaces is given. Various anchor groups designed to connect organic materials to metal electrodes are presented (e.g. thiolates, dithiocarbamates, mercuryls and stannyls) and their potential for optimizing the charge injection as well as the morphological, chemical, and electronic nature at the contact is illustrated. On this basis, functional molecular building blocks are grafted to the surface by self-assembly, providing rectification, switching, or chemical selectivity. Once the key parameters for interface formation and fabrication are under control, a huge number of potential applications emerge, ranging from optoelectronics to organic printed circuits. As one example, electrostatic dipole layers for tuning the injection barrier between metals and organic semiconductors are presented, which may find applications in organic light emitting diodes, field effect transistors, and solar cells. When further reducing device dimensions towards the nanoscale, organic monolayers might foster the development of molecular electronics, as illustrated here by highly robust metal-molecule-metal junctions based on FeII-terpyridine molecular wires or by optically switchable protein layers.

TT 10.2 Mon 9:45 H 2032

Grain boundaries in $CuInSe_2$ and $CuGaSe_2$ solar cell materials: New insights from hybrid functional calculations — Hossein Mirhosseini, •Janos Kiss, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.

Polycrystalline thin-film solar cells based on $CuIn_{1-x}Ga_xSe$ (CIGSe) are an economically viable alternative to the Si based technology. During the deposition of the polycrystalline light absorber layer grain boundaries (GBs) are formed in the CIGSe material, and the effect of these GBs upon the structural and electronic properties of the thin-film solar cells are not yet fully understood. Different atomic structures of the GBs in CIGSe have been reported experimentally. The outcomes of the theretical calculations, however, are diverse and sometimes inconsistent due to the limitation of the functionals, which fail to properly describe the band gap of thin film solar cell materials. Employing a state of the art method using the HSE hybrid functional, which is known to predict the atomic and electronic structure of solar cell materials rather well, we have looked at the behavior and properties of GBs in $CuInSe_2$ and $CuGaSe_2$. In the framework of our investigation, we have studied the atomic relaxation and electronic structure of various GBs and also considered the effect of the impurity segregation close to the GBs.

TT 10.3 Mon 10:00 H 2032

Relationship between the chemical structure of low band gap polymers and self-organization properties — •Milutin Ivanovic[1], Umut Aygül[1], Ulf Dettinger[1], Aurelien Tournebize[1], David Batchelor[2], Stefan Mangold[2], Heiko Peisert[1], and Thomas Chassé[1] — [1]) University of Tuebingen, Institute of Physical and Theoretical Chemistry, 72076 Tuebingen, Germany — [2]Karlsruhe Institute of Technology (KIT), ANKA Synchrotron Radiation Facility, 76344 Eggenstein-Leopoldshafen, Germany

A possible approach to improve the efficiency of donor-acceptor based bulk heterojunction (BHJ) of OPV cells is the use of low band gap (LBG) polymers as donor materials. Basic electronic processes in OPV cells are however strongly influenced by the morphology and the ability for self-organization of the polymers in the thin-films. We utilize NEXAFS spectroscopy to study the molecular orientation of novel LBG polymers (PCPDTTBBTT, PCPDTTBTT and PCPDTzTBTT) for OPVs in thin films. The influence of post-processing annealing as well as of blending with Phenyl-C61-butyric acid methyl ester (PCBM) on the orientation is investigated. The studied LBG polymers are characterized by a variation of (hexyl-) thiophene groups compared to related LBG polymers recently studied.[1,2]. Acknowledgments: This research is funded by the European Union Seventh Framework Programme (FP7/2011 under grant agreement ESTABLIS n° 290022). References: 1.*Aygül, U. et al. J. Phys. Chem. C 2012, 116, 4870-4874. 2.*Aygül, U. et al. Sol. Energ. Mat. Sol. Cells 2014, 128, 119-125.

TT 10.4 Mon 10:15 H 2032

Organic ambipolar field-effect transistors: *In situ* electrical investigation of MnPC-OFETs — •Franziska Lüttich, Ovidiu D. Gordan, and Dietrich R. T. Zahn — Semiconductor Physics, Technische Universität Chemnitz, Chemnitz, Germany

On the way to low-cost and flexible applications organic semiconducting materials are promising. Devices like organic light-emitting diodes, organic solar cells, and organic field-effect transistors (OFETs) can be produced *e.g.* on flexible and elastic substrates and with chemical variation of side groups or substitution of metal centers their properties like optical absorption and charge carrier mobilities can be influenced.

Here we present a temperature dependent study on Manganese Phthalocyanine (MnPc)-OFETs, which reveal an ambipolar behaviour. In order to investigate the electrical properties of MnPc we used OFET "'end-of-line"' substrates from Fraunhofer IPMS with a 100 nm thick thermal silicon dioxide layer as dielectric. The investigated bottom-contact OFETs were fabricated under high vacuum conditions ($p < 4 \cdot 10^{-7}$ mbar) by evaporating MnPc on top of the pre-structured substrates. The electrical DC characteristics were measured *in situ* as a function of temperature. This procedure enables us to determine the activation energies for the hole and electron transport. The influence of ambient atmosphere was also investigated and revealed strong impact on the electrical performance. The topography was determined using an Atomic Force Microscope (AFM).

TT 10.5 Mon 10:30 H 2032

Photoelectron spectroscopy studies on efficient air-stable molecular n-dopants — •Martin Schwarze[1], Max L. Tietze[1], Paul Pahner[1], Ben Naab[2], Zhenan Bao[2], Björn Lüssem[1], Daniel Kasemann[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Chemical Engineering, Stanford University, Stanford, California 94305, United States

Understanding the working mechanism of electrical doping in organic semiconductors is essential for the optimization of organic semiconductor devices such as organic light emitting diodes or organic solar cells. A defined doping concentration allows for the control of the Fermi-level position as well as the adjustment of the conductivity of transport layers. In comparison to molecular p-doping of organic semiconductors, n-doping creates the additional problem of air instability. To successfully transfer an electron to the lowest unoccupied molecular orbital (LUMO) of the matrix material, dopants exhibiting shallow highest molecular orbitals (HOMO) are necessary, rendering them prone to reactions with e.g. oxygen. In this study, three different types of n-dopants are compared: air stable cationic DMBI dopants, halogen-free DMBI dimers, and the established but air sensitive Cr2(hpp)4. Fermi-level shift and conductivity of co-evaporated Bis-HFl-NTCDI layers at different doping concentrations as well as stability during air exposure are investigated by UPS and electrical measurements.

TT 10.6 Mon 10:45 H 2032

Mode-selective vibrational manipulation of charge transport in π-conjugated molecular materials — •Robert Lovrincic[1,2], Artem A. Bakulin[3,4], Yu Xi[1], Oleg Selig[3], Huib J. Bakker[3], Yves L. A. Rezus[3], Pabitra K. Nayak[1], Alexandr Fonari[5], Veaceslav Coropceanu[5], Jean-Luc Bredas[5,6], and David Cahen[1] — [1]Department of Materials & Interfaces, Weizmann Institute of Science, Israel — [2]IHF, TU Braunschweig & Innovationlab, Germany — [3]FOM Institute AMOLF, The Netherlands — [4]Cavendish Laboratory, University of Cambridge, UK — [5]School of Chemistry and Biochemistry , Georgia Institute of Technology, USA — [6]Solar & Photovoltaics Center, King Abdullah University, Saudi Arabia

The soft character of organic materials leads to strong coupling between molecular nuclear and electronic dynamics. This coupling opens the way to control charge transport in organic electronic devices by directing molecular vibrational motions. However, despite encouraging

theoretical predictions, experimental realization of such control has remained elusive. Here we demonstrate experimentally that photoconductivity in a model organic optoelectronic device can be controlled by the selective excitation of molecular vibrations. Using an ultrafast infrared laser source to create a coherent superposition of vibrational motions in a pentacene/C60 photoresistor, we observe that excitation of certain modes in the $1500-1700\,\mathrm{cm}^{-1}$ region leads to photocurrent enhancement. The effect depends on the nature of the vibration and its mode-specific character can be well described by the vibrational modulation of intermolecular electronic couplings.

TT 10.7 Mon 11:00 H 2032

Investigation of charge transfer in organic semiconductors using infrared spectroscopy — •Tobias Glaser[1,2], Sebastian Beck[1,2], and Annemarie Pucci[1,2,3] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik — [2]InnovationLab GmbH, 69115 Heidelberg — [3]Universität Heidelberg, Centre for Advanced Materials

Charge transfer in organic semiconductors is used in various ways to increase the performance of organic electronic devices. For example electrochemical doping is used to increase the conductivity in charge transport layers. Additionally, charge injection layers are used to decrease injection barriers between electrodes and organic transport layers. In both cases molecular charge transfer plays an important role, but the basic mechanisms are still subject of heated debate. Due to strong relaxation effects upon molecular charging, infrared (IR) spectroscopy is very well suited to investigate charge transfer in organic semiconductors. Neutral and charged molecules can be distinguished by their different specific vibrational features in spectra of doped layers as well as for interfaces. In this study we investigated charge transfer in thin layers of commonly known transport materials such as 4,4*-bis(N-carbazolyl)-1,1*-biphenyl (CBP) doped with inorganic and organic dopants such as MoO3 or F4TCNQ and at interfaces of organic semiconductors. By quantitative analysis of the experimental spectra the doping efficiency and the degree of charge transfer can be determined for the doped layers. Whereas, for interfacial charge transfer, the formation of a space charge region can be mapped. Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

TT 10.8 Mon 11:15 H 2032

Structure and Photovoltaic Performance of Chiral Anilino Squaraines — •Manuela Schiek[1], Matthias Schulz[2], Stefanie Brück[1], Martin Silies[3], Heiko Kollmann[3], Christoph Lienau[3], Arne Lützen[2], and Jürgen Parisi[1] — [1]Energy and Semiconductor Research Laboratory, University of Oldenburg, Germany — [2]Kekule-Institute for Organic Chemistry and Biochemistry, University of Bonn, Germany — [3]Ultrafast Nano-Optics, University of Oldenburg, Germany

Small molecular semiconductors such as squaraines are advantageous compared to polymeric materials because they allow a more direct control of the structure on the molecular level and consequently solid state properties. Especially the implementation of chiral side chains introduces new functionalities such as circular dichroism. Different 1,3-bis(N,N-substituted-2,6-dihydroxy-anilino)squaraines with varying terminal N-substitution, in some cases including a stereogenic center, are investigated as single crystals, in thin films and blended with a fullerene acceptor as active layer in bulk heterojunction organic solar cells.

TT 10.9 Mon 11:30 H 2032

Charge separation and C_{60} crystallinity in bulk heterojunction solar cells: the decisive role of device architecture — •Felix Schell[1,2], Michael Scherer[1,3], Diana Nanova[1,2,3], Anne Katrin Kast[2,4], Wolfgang Kowalsky[1,2,3], Rasmus R. Schröder[1,4,5], and Robert Lovrincic[1,3] — [1]InnovationLab GmbH, Heidelberg — [2]Kirchhoff-Institute for Physics, Heidelberg University — [3]Institute for High-Frequency Technology, TU Braunschweig — [4]CellNetworks, BioQuant, Heidelberg University — [5]Center for Advanced Materials, Heidelberg University

The crucial influence of C_{60} crystallinity on the charge separation in organic solar cells (OSC) has been realized very recently. Here, we show the importance of the device architecture on C_{60} crystallisation in the bulk-heterojunction (BHJ). Active layer morphology of small molecule BHJ OSC and its influence on device performance are studied by means of energy-filtered transmission electron microscopy (EFTEM) and electrical characterization. The influence of substrate temperature during deposition and of pure sublayers is assessed. BHJs fabricated at room temperature are found to be finely mixed and amorphous, whereas the corresponding films deposited onto heated substrates show pronounced phase separation. Despite these clear morphological changes, substrate heating does not increase efficiency of OSCs in a non-inverted device architecture. Improvements found in literature for inverted cells can be attributed to stronger acceptor crystallization, present, if deposited onto a pure C_{60} layer but not with an F_4ZnPc substrate, leading to more efficient exciton dissociation.

TT 10.10 Mon 11:45 H 2032

Influence of DMSO-treatment on morphology, composition and performance of PEDOT:PSS layers in organic photovoltaic cells — Sidhant Bom, •Torsten Balster, Marlis Ortel, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

PEDOT:PSS layers in organic solar cells are used as hole transport (HTL) and electron blocking layers. Therefore the morphology and composition of the layer and the interface have a great influence on the performance of organic photovoltaic devices.

Additional post-deposition treatment of the PEDOT:PSS layers (HTL) in P3HT/PCBM solar cells were studied in this work. For this purpose, pristine PEDOT:PSS layers were spin coated with dimethyl sulfoxide (DMSO) after annealing. Pristine and treated layers were characterized by means of electrical characterization, atomic force microscopy (AFM) and x-ray photoelectron spectroscopy (XPS).

The additional post-deposition DMSO treatment induces an increase in power conversion efficiency by more than 50%. In addition, the open circuit voltage and the short-circuit current were enhanced, whereas the fill factor remained constant. This behavior is explained by modification of the PEDOT:PSS-semiconductor interface. On the one hand smoothening of the interface by reduction of large PSS particles visible in AFM occurs. On the other hand XPS data show a reduction of PSS-sulphur species. Less PSS at the interface should improve the charge carrier injection properties, as observed experimentally.

TT 10.11 Mon 12:00 H 2032

Charge transfer, optical and transport properties in pure organic heterostructures — •Liebing Simon, Hahn Torsten, and Kortus Jens — Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Strasse 23, 09599 Freiberg

We will present theoretical investigation on pure charge transfer materials within the density functional theory framework (DFT). Starting from the recently fabricated picene-F_4TCNQ [1] we explore the electronic and optical properties of novel representatives of this new class of materials. These representatives are formed of polycyclic hydrocarbons and TCNQ derivatives and we compare our results with experimental spectroscopic data.

The picene-F_4TCNQ system shown pronounced diode transistor behavior [2]. By means of DFT/NEGF (non equilibrium green function formalism) [3,4] we obtain the IV-characteristics of selected model devices for these systems. The formation of hybrid orbitals together with intrinsic charge transfer seems to be the origin of the novel electronic and transport properties [5].

[1] Mahns, B. et. al. Crystal Growth & Design (2014). [2] Hahn T., Liebing S., and Kortus J., Nanoscale 6, 14508 (2014). [3] Pederson, M. et. al. Phys. Status Solidi b 217, 197. (2000) [4] Enkovaara, J. et al. Journal of Physics: Condensed Matter 22, 253202 (2010). [5] Lindner S. et. al. Phys. Rev. Lett. 109, 027601 (2012).

TT 10.12 Mon 12:15 H 2032

Single molecule circuits with N-heterocyclic carbene linkers — •Hector Vazquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

In single molecule circuits, where an electrical current flows through a molecule, conducting molecules often have terminal linker groups which bind to the metallic electrodes [1]. These chemical link groups strongly influence the conducting properties, often acting as bottlenecks for electron transmission and result in low-transmission resonances localized at the interface. Therefore, identifying adequate chemical linker groups is essential for achieving ideal mechanical and conducting properties in molecular circuits.

Recently, SAMs of N-heterocyclic carbenes on gold were shown to have very high thermal and oxidative stability [2], making N-heterocyclic carbenes potentially very useful linkers for single molecule transport. In this talk, I will present results from first-principles simulations based on DFT-NEGF for the electronic and conducting properties of carbene-terminated molecules. I will show results for the adsorption properties of N-heterocyclic carbenes on gold. I will also

present transmission calculations of carbene-terminated molecules and discuss these results in the context of other metal-molecule links with Au-C bonds [3].

[1] F. Schwarz and E. Loertscher, J. Phys. Condens. Matter 26 474201 (2014).
[2] C.M. Crudden et al., Nature Chemistry 6 409 (2014).
[3] W. Chen et al., J. Am. Chem. Soc. 133 17160 (2011).

TT 10.13 Mon 12:30 H 2032

Charge and spin transfer materials for molecular electronic and spintronic applications — •Torsten Hahn, Simon Liebing, and Jens Kortus — TU Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg

The combination of different functionalized metal phthalocyanines was found to lead to novel charge- and spin transfer compounds [1,2]. The recently synthesized picene / F4TCNQ charge transfer salt [3] also shows promising physical properties and the theoretical modeling predicts the material to act as a molecular diode with high rectification ratio [4]. Based on density-functional theory calculations we show that in case of the metal phthalocyanines as well as for the picene / F4TCNQ system hybrid states formed by the donor / acceptor system are playing the key role to determine the spectroscopic and quantum transport properties. We further conclude that the tuning of quantum transport properties through hybrid states is a general concept which opens a new route towards functional materials for molecular electronics.

[1] R. Friedrich et al., Phys. Rev. B 87, 115423 (2013). [2] R. Friedrich, B. Kersting, and J. Kortus, Phys. Rev. B 88, 155327 (2013). [3] Mahns, B. et. al., Cryst. Growth and Design 14, 1338-1346 (2014). [4] T. Hahn, S. Liebing, and J. Kortus, Nanoscale 6, 14508 (2014).

TT 10.14 Mon 12:45 H 2032

Device-like calcium corrosion test for ultra-barrier materials — •Frederik Nehm[1], Hannes Klumbies[1], John Fahlteich[2], Felix Dollinger[1], Karl Leo[1], and Lars Müller-Meskamp[1] — [1]Institut für Angewandte Photophysik, TU Dresden, Dresden, Deutschland — [2]Fraunhofer FEP, Dresden, Deutschland

The continuous progress of organic electronics demands for flexible moisture barriers with water vapor transmission rates (WVTRs) below $10^{-4}\ \frac{g(H_2O)}{m^2 d}$ and quick, reliable measurement techniques for such WVTRs. The electrical calcium corrosion test is an extremely sensitive technique used widely in research groups. However, setups differ strongly as do their accuracy and background rates. We report on common issues and show how we manage them in our setup. Barrier corrosion because of direct water condensation on its surface is prevented by a glued-on PET film and Ca-induced stress is mitigated by organic decoupling layers. We demonstrate the effectiveness of our approach with studies on sputtered Zinc-Tin-Oxide and atomic layer deposited (ALD) alumina moisture barriers in different aging climates. Single barriers show a linear WVTR increase with rising absolute humidity at given temperature. Below $40°C$, this is even valid independent of temperature. A divergence at higher temperatures probably originates from the actual barrier layer, since this effect cannot be observed for the pure substrate. Also, nanolaminates using ALD alumina, titania and alkoxide, and multilayer barriers with polymer interlayers with WVTRs down to at least $2 \cdot 10^{-5}\ \frac{g(H_2O)}{m^2 d}$ in $38°C$, 90% relative humidity environments are investigated.

TT 11: Magnetic Heuslers, Half-Metals and Oxides (jointly with MA)

Time: Monday 9:30–12:45 Location: H 0112

TT 11.1 Mon 9:30 H 0112

Half-metallic compensated ferrimagnetic behaviour of $Mn_{1.5}V_{0.5}$FeAl Heusler compound — •Rolf Stinshoff, Peter Adler, Gerhard Fecher, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Half-metals, i.e. materials exhibiting 100 % spin polarization, naturally attract much interest in spintronics [1]. Some of them have already shown their potential in applications such as magnetic tunneling junctions. Despite the very high TMR ratios achieved at low temperatures using half-metallic materials, further technological requirements, such as low stray fields, temperature stability etc., still have to be improved. In this context, some advantages are provided by the group of completely compensated ferrimagnets which still keep the half-metallicity. Several of them were predicted theoretically within the Heusler family. Here we will discuss the experimentally measured characteristics (structural, magnetic and transport properties) of the newly synthesized $Mn_{1.5}V_{0.5}$FeAl Heusler material, which is suggested to be a fully compensated half-metallic ferromagnet by the first principle calculations [2].

[1] R. A. de Groot, F. M. Müller, P. G. van Engen, K. H. J. Buschow, Phys. Rev. Lett. **50**, 2024-2027 (1983)
[2] S. Wurmehl, H. C. Kandpal, G. H. Fecher, C. Felser, J. Phys. Condens. Matter **18**, 6171-6181 (2006)

TT 11.2 Mon 9:45 H 0112

High-throughput screening for antiferromagnetic Heusler compounds using density functional theory — •Jan Balluff, Markus Meinert, and Günter Reiss — Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany

Due to the exchange bias effect, antiferromagnetic compounds are of particular interest for the field of spintronics. Since Heusler compounds are a very versatile family of alloys, we attempt to find promising antiferromagnetic compounds unknown by now. We report on a high-throughput screening among the Heusler compounds for stable antiferromagnetic systems. Starting from a detailed evaluation of raw magnetic data for Heusler compounds extracted from the AFLOWLib [1], we extend the data by explicitly checking for stable antiferromagnetic ground states. [1] S. Curtarolo et al., Comp. Mat. Sci. 58 , 218 (2012)

TT 11.3 Mon 10:00 H 0112

Spin-selective electron localization induced by disorder in Mn-Co-Al Heusler alloys — •Sunil Wilfred D'Souza, Siham Ouardi, Lukas Wollmann, Stanislav Chadov, and Claudia Felser — Max-Planck-Institut für Chemische Physik fester Stoffe

Understanding the role of disorder opens new alternatives in the state-of-the-art design of the multicomponent materials. First proposals to improve the electron transport characteristics by constructive chemical disorder were already suggested for the tetragonal non-halfmetallic ferrimagnetic Mn_3Ga-based Heusler alloys, where the possibility of the spin-selective electron localization was demonstrated by the first-principles. Here we consider the spin-selective electron localization within the cubic $Mn_{2-x}Co_{1+x}Al$ ($0 \leq x \leq 1$) Heusler series. In contrast to the strongly anisotropic tetragonal case, the isotropic cubic geometry allows for an easier experimental check of the proposed spin-selective electron localization. The residual transport properties, i.e. spin-projected resistivities were calculated within the Kubo-Greenwood linear response formalism, using Coherent Potential Approximation (CPA) description for the electron localization, within the framework of the fully-relativistic SPR-KKR Green's function method. Here we also give the comparison with the first experimental data.

TT 11.4 Mon 10:15 H 0112

Advantages of constructive disorder: design of the spin-selective electron localization in Mn_3Ga-derivatives — •Stanislav Chadov, Sunil Wilfred D'Souza, Lukas Wollmann, and Claudia Felser — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

Understanding the role of disorder opens new alternatives in the state-of-the-art design of the multicomponent materials. Theoretically we will try to design a situation in which the constructive disorder serves as a mechanism preventing the propagation of certain quasiparticles, namely the spin-down electrons – the so-called *spin-selective* electron localization. Here we make use of chemical disorder induced by the small stoichiometric variations. As a suitable example, we take a non-halfmetallic Mn_3Ga Heusler, and subsequently develop the appropriate constructive disorder scheme justifyed by the first-principles calculations based on the Coherent Potential Approximation (CPA) and Kubo-Greenwood linear response formalsim within the framework of the SPR-KKR Green's function method. As it follows from our

results, almost any relatively small substitution of Mn by other 3*d* transition element (except of Cu) leads to a dramatic increase of the spin-polarization along the tetragonal crystalline axis.

TT 11.5 Mon 10:30 H 0112

Superconducting TiN seed layer for Heusler compounds — •Alessia Niesen[1], Manuel Glas[1], Daniel Ebke[2], Jan Schmalhorst[1], and Günter Reiss[1] — [1]Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

TiN thin films were prepared by DC and RF magnetron sputtering in an UHV sputtering system. Epitaxial growth was achieved on MgO (001) and $SrTiO_3$ (001) substrates at deposition temperatures above 450°C. The crystallographic and surface properties of TiN were determined by X-ray diffraction (XRD) and reflection (XRR) measurements. In addition, atomic force microskopy (AFM) was performed to verify the low roughness ($< 1\,nm$) measured by the XRR. The out-of-plane lattice constant and the resistivity of TiN reached the theoretical predicted values of 4.24 Å and nearly $20\,\mu\Omega cm$ (bulk value). 4-terminal transport measurements in a closed cycled helium cryostat showed a phase transition to the superconducting state at temperatures below 5 K for TiN deposited at 450°C on MgO and $SrTiO_3$ substrate. The suitability of TiN as seed layer for ferromagnetic materials like Iron and Heusler compounds, e. g. Co_2FeAl and $Mn_{3-x}Ga$, was investigated by analysing the crystallographic and magnetic properties. Epitaxial growth of both Heusler compounds (Co_2FeAl and $Mn_{3-x}Ga$) on a TiN seed layer has been proven for various deposition temperatures. Hall-measurements additionally showed a higher coercitivity and squareness ratio for Mn-Ga thin films when prepared on a TiN buffer.

TT 11.6 Mon 10:45 H 0112

Mn-based candidates for rare earth free permanent magnet — •Adel Kalache, Bayardulam Jamiyansuren, Siham Ouardi, Guido Kreiner, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Permanent magnets are used in a wide range of applications from hybrid cars and wind turbines to computer hard-disk drives. Rare earth (RE) magnets such as Nd-Fe-B and Sm-Co show unique hard magnetic performance but are subject to both price and supply issues. New RE free permanent magnets are also needed to fill the gap between the low cost hexagonal ferrites and the expensive RE magnets. Some Mn-based intermetallic compounds are promising candidates because of their high Curie temperature and their tetragonal structure of the $L1_0$ type or distorted Heusler $D0_{22}$ type. The resulting intrinsic uniaxial magnetic anisotropy leads to appreciable hard magnetic properties. The synthesis of Mn-based RE free magnets with melt spinning technique improves some extrinsic properties such as microstructure and grain size. These features allow an increase of the coercivity of material, leading to higher figure of merit BH_{max}. Structural characterization and magnetic properties of some tetragonal Mn-based compounds such as Mn-Ga and Mn-Ge will be presented. Neutron diffraction is reported for $Mn_{60}Ga_{40}$. Substitution of Mn with other transition metals will also be discussed in order to improve the magnetic hardness.

15 min. break

TT 11.7 Mon 11:15 H 0112

Calculation of electronic structure and field-induced magnetic collapse in ferroic materials — •Peter Entel — Faculty of Physics, University Duisburg-Essen, D-47048 Duisburg, Germany

We have performed ab initio electronic structure calculations and Monte Carlo simulations of Fe-Rh, Mn-Ga-C and Heusler intermetallics alloys such as Ni-Co-Cr-Mn-(Ga, In, Sn) which are of interest for magnetic shape-memory devices, solid-state refrigeration and energy systems, an emerging technology involving solid systems. The calculations reveal that the important magnetic phase diagrams of these alloys which show the magnetic collapse and allow predictions of the related magnetocaloric effect which they exhibit at finite temperatures, can be obtained by the ab initio computations alone. This is a one-step procedure from theory to alloy design of ferroic functional devices.

TT 11.8 Mon 11:30 H 0112

Ab initio study of tetragonal Heusler alloys for magnetic applications with high anisotropies — •Heike C. Herper, Yaroslav O. Kvashnin, and Olle Eriksson — Department of Physics and Astronomy, Uppsala University, Sweden

Materials with high magnetic anisotropy (MAE) are of broad technological interest whereby typical magnets with high MAE are based on expensive materials such as Pt or Nd. Therefore, cheap and abundant replacements are demanded. Heusler alloys are of special interest because their magnetic and structural properties can be quite easily designed by composition. Here we present an ab initio study for a series of tetragonal Ni-based Heusler alloys Ni_2YZ with (Y = Mn, Fe, Co) and Z varying from B to Sn. Combined VASP and RSPt investigations reveal MAE values for $L2_1$ ordered Co containing alloys which are comparable to the Mn-Ga based alloys found in literature. However, for e/a values larger than 32 they tend to inverse order which is accompanied by a significant reduction of the MAE. Even though the MAE values for alloys with Y = Fe are found to be smaller compared to the Ni_2CoZ alloys, the maximum energy products are similar. In contrast to the $L2_1$ ordered Ni_2CoZ systems out of plane MAE has been observed for several Ni_2FeZ alloys.

TT 11.9 Mon 11:45 H 0112

Magnetism in tetragonal Heusler compounds — •Lukas Wollmann[1], Stanislav Chadov[1], Jürgen Kübler[2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany. — [2]Institut für Festkörperphysik, Technische Universität Darmstadt, Darmstadt, Germany

Compounds with uniaxial anisotropy are of general interest in the field of magnetism, and in particular within the emerging field of spintronics. Uniaxial anisotropy is an inherent property of many tetragonal Heusler compounds. Here we report on a comprehensive study on tetragonal Manganese-based Heusler compounds, by starting from a set of cubic parent systems and continuing with the mechanisms of their tetragonal distortion, in particular focusing on the magnetic properties, and explaining the microscopic origin of the observed properties, as for example, for the magnetocrystalline anisotropy. Rather high anisotropy values were obtained for those systems containing heavy transition metals, which suggests them as candidate materials for spin transfer torque magnetization switching applications.

TT 11.10 Mon 12:00 H 0112

Phase separation in NiSn- and CoSb-based Half-Hesleur alloys — Joaquin Miranda Mena, •Heiko G. Schoberth, Thomas Gruhn, and Heike Emmerich — Material- und Prozesssimulation, Bayreuth University. Universitätsstraße 30 D-95448 Bayreuth, Germany

We combine DFT calculations, Monte Carlo simulations and mean field models to study the thermodynamic conditions for phase separation in two families of quaternary-Half-Heusler alloys. In the first family, γNiSn (γ =TiHf, TiZr), we found that phase separation is achieved in the range 500-700 K, but no phase separation is present when alloying with γ=ZrHf. For CoTi(1-x)ZxSb (Z=Sc, Cr, Mn, Fe, Cu) we found transition temperatures in the range 800-3000 K. The transition temperature is favored at nearly one third of concentration (x). However, at large x some materials do not present phase separation, but rather a type of crystal order. We discuss these results in the view of thermoelectrics, where apparently induced phase separation enhances the figure of merit.

TT 11.11 Mon 12:15 H 0112

Highest Curie temperature in Co-Fe based Heusler compounds — •Julia Erika Fischer[1], Siham Ouardi[1], Gerhard Fecher[1], Guido Kreiner[1], Peter Adler[1], Claudia Felser[1], Simone Fabbrici[2], and Franca Albertini[2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Institute of Materials for Electronics and Magnetism CNR, Parma, Italy

Half-metallic ferromagnetic Co-based Heusler compounds are one of the most promising class of materials for high performance spintronic devices due to the recently experimentally demonstrated strong spin polarization and their reported high Curie temperatures [1, 2].
We have prepared a series of polycrystalline Co-Fe based Heusler alloys and studied the structural and magnetic properties. From thermomagnetic analysis measurements we found Curie temperatures of more than 1200 K, which are the highest values in Heusler alloys so far. Therefore, a higher thermal stability of magnetization is expected even for moderate device temperatures. In particular, the Co-Fe disorder was

investigated by Mößbauer spectroscopy to study the influence on the magnetic properties.

[1] B. Balke et al., Sci. *Technol. Adv. Mater.* 9, 014102 (2008).
[2] M. Jourdan et al., *Nat. Commun.*, 5 (3974), 1 (2014).

TT 11.12 Mon 12:30 H 0112

Antiferromagnetic order in CuMnSb crystal and its stability — •Frantisek Maca, Vaclav Drchal, and Josef Kudrnovsky — Institute of Physics ASCR, Praha, Czech Republic

It is well known that the ground state of the CuMnSb is antiferromagnetic with alternating ferromagnetic layers in the <111> direction - the AFM(111) structure. The first ab initio calculations comparing nonmagnetic, ferromagnetic and AFM(111) structures [1] also have shown that the antiferromagnetic state has the lowest total energy. However, we found by using FLAPW and TB-LMTO calculations that the ideal AFM(001) structure has always lower total energy than the AF(111).

Experimental measurements show a high resistivity of CuMnSb samples which indicates the presence of disordered impurities. We compare formation energies for various defects in order to find the type of disorder which favors the AFM arrangement. Calculations indicate as the most probable candidate the Mn-Cu swapping. We show that presence of disorder and electron correlations are needed for realistic theoretical description. The total energy results are supported by discussion of magnetic exchange interactions.

[1] T. Jeong, Ruben Weht, and W. E. Pickett, Phys. Rev. B 71, 184103 (2005).

TT 12: Graphene: THz, NIR, and Transport Properties (jointly with HL, O)

Time: Monday 9:30–11:30 Location: ER 270

TT 12.1 Mon 9:30 ER 270

Ratchet effects in graphene with a lateral periodic potential — •P. Olbrich[1], J. Kamann[1], J. Munzert[1], M. König[1], L.E. Golub[2], L. Tutsch[1], J. Eroms[1], F. Fromm[3], Th. Seyller[3], D. Weiss[1], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Technical University of Chemnitz, Germany

We report on the observation of terahertz (THz) radiation induced photocurrents in (a) epitaxially grown and (b) exfoliated graphene with a lateral periodic potential. The samples were covered with an insolating layer and a sequence of asymmetrically spaced thin/thick metallic stripes. While in the reference of sample (a) under normal incidence of THz radiation no photosignal was observed, the illumination of the lateral periodic potential resulted in pronounced photosignals, consisting of polarization dependent and independent contributions. In case of sample (b) the thin/thick metallic stripes act as a dual top gate structure to vary the potential profile and a back gate allows to change the carrier type and density of the sample. Here, the photocurrent reflects the degree of asymmetry induced by different top gate potentials and even vanished for a symmetric profile. Moreover, around the Dirac point the photocurrent shows strong oscillation. We discuss the experimental data, taking into account the calculated potential profile, near field effects of light scattering and the theoretical model [1, 2].

[1] E. L. Ivchenko and S. D. Ganichev, JETP Lett. 93, 673 (2011).
[2] P. Olbrich et al., Phys. Rev. B 83, 165320 (2011).

TT 12.2 Mon 9:45 ER 270

Mechanically Modulated Graphene for THz-Nanoelectronics. — •Jonas Sichau[1], Timothy Lyon[1], August Dorn[1], Amaia Zurutuza[2], Amaia Pesquera[2], Alba Centeno[2], and Robert Blick[1] — [1]Center for Hybrid Nanostructures, Institutes of Nanostructure and Solid State Physics, University of Hamburg, Jungiusstrasse 11c, 20355 Hamburg, Germany. — [2]Graphenea S.A., 76 Tolosa Hiribidea, Donostia-San Sebastian, E-20018, Spain.

Graphene offers very high charge carrier mobility and a mean free path of several microns at room temperature. Consequently, it is a promising material for THz electronics [1]. For flat monolayer graphene, studies on microwave-photo excited transport have found spin resonance and zero-field pseudo-spin splitting [2]. The aim of our work is to investigate spatially modulated graphene under microwave excitation. Once carriers are propagating ballistically through the undulated graphene sheet, it is predicted that THz-radiation should be emitted [1].

We fabricated extremely large graphene membranes of up to 1 mm side lengths and transferred these onto a SiO_2-substrate. The pitch and height of the mechanical modulation are of the order of 200 nm and 50 nm, respectively. The measurements are performed with a variable temperature insert (VTI) at magnetic fields up to 12T. The microwave signal is coupled to the sample via a micro inductor forming a resonator with the graphene sheet. With this configuration we are able to probe magnetotransport and the interaction with electromagnetic radiation.

[1] Tantiwanichapan et al., Nanotechnology 24, 375205 (2013)
[2] Mani, R.G. et al., Nat. Commun., 3:996 (2012)

TT 12.3 Mon 10:00 ER 270

Investigations on the polarization dependent carrier excitation in graphene with low energetic photons — •Jacob Otto[1,2], Martin Mittendorff[1,2], Torben Winzer[3], Ermin Malic[3], Andreas Knorr[3], Harald Schneider[1], Manfred Helm[1,2], and Stephan Winnerl[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Technische Universität Berlin, 10623 Berlin, Germany

We demonstrate that in graphene a nonequelibrium charge carrier distribution retains its anisotropic nature on a 10 ps timescale if the photon energy is below the optical phonon energy. Recently evidence for an anisotropic carrier distribution has been found in near-infrared pump-probe experiments with varied angle between the orientation of pump and probe polarization [1]. This anisotropy vanishes after 150 fs due to electron optical-phonon scattering. Extending this study to the mid-infrared range (E_{Photon} = 74 meV), i.e. to energies below the optical phonon energy, allows to strongly suppress this scattering mechanism. In accord with microscopic theory, traces of an anisotropic distribution on a 10 ps timescale are found. Note that carrier-carrier scattering, acting on a 10 fs timescale, is mainly colinear and therefor preserves the anisotropic distribution on rather long timsecales.

[1] M. Mittendorff, T. Winzer, E. Malic, A. Knorr, C. Berger, W. A. de Heer, H. Schneider, M. Helm and S. Winnerl *Nano Lett.* 2014, 14, 1504-1507

TT 12.4 Mon 10:15 ER 270

Magnetotransport in small angle twisted bilayers of folded graphene — •Johannes Rode[1], Hennrik Schmidt[1,2], Dmitri Smirnov[1], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore

Naturally occurring double-layer graphene consists of two hexagonal lattices in Bernal-stacking, described by a translational displacement between layers. While this type of bilayer is most commonly studied, the introduction of a rotational mismatch opens up a whole new field of rich physics, especially at small interlayer twist[1,2]. We investigate magnetotransport measurements on twisted graphene bilayers, prepared by folding of single layers. These reveal a strong dependence on the twist angle, which can be estimated by means of sample geometry. At small rotation, superlattices with a wavelength in the order of 10 nm arise and are observed by friction atomic force microscopy. Magnetotransport measurements in this small-angle regime show the formation of satellite Landau fans, which are attributed to additional Dirac singularities in the band structure[3].

[1] Lopes dos Santos, J. M. B., Peres, N. M. R. & Castro Neto, A. H. *Phys. Rev. Lett.* **99**, 256802.
[2] Mele, E. J. *Phys. Rev. B* **84**, 235439.
[3] Schmidt, H., Rode, J. C., Smirnov, D. & Haug, R. J. *Nat. Commun.* (accepted, Nov. 2014).

TT 12.5 Mon 10:30 ER 270

Carrier dynamics in Landau-quantized graphene — •Florian Wendler[1], Martin Mittendorff[2], Stephan Winnerl[2], Manfred Helm[2], Andreas Knorr[1], and Ermin Malic[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

We investigate the carrier dynamics in Landau-quantized graphene after an optical excitation using microscopic time-resolved calculations as well as differential transmission measurements. The calculations are performed within the density matrix theory accounting for the carrier-light, carrier-carrier, and carrier-phonon interaction which allows for a microscopic explanation of the experimental spectra.

The energy spectrum of Landau-quantized graphene is characterized by non-equidistant Landau levels where the optical selection rules enable a selective excitation of specific transitions. This is exploited to investigate the carrier dynamics in the energetically lowest Landau levels where an unexpected sign reversal in pump-probe spectra, observed in experiment and theory, provides an evidence for strong Auger scattering [1]. Based on our calculations we predict a substantial carrier multiplication [2]. Furthermore, the theory reveals the occurrence of population inversion in Landau-quantized graphene, suggesting its application as gain medium for a widely tunable Landau level laser[3].

[1] M. Mittendorff et al., Nat. Phys., DOI:10.1038/nphys3164.
[2] F. Wendler et al., Nat. Commun. 5:3703 (2014).
[3] F. Wendler, and E. Malic, arXiv:1410.2080v1.

TT 12.6 Mon 10:45 ER 270

Giant magnetophotoelectric effect in suspended graphene — •Jens Sonntag, Annika Kurzmann, Martin Geller, Ralf Schützhold, and Axel Lorke — Faculty of Physics and CeNIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Due to the broad absorption bandwidth and the possibility for carrier multiplication, graphene is a promising candidate for optoelectric applications.

In this context, we performed photocurrent measurements on a suspended graphene field-effect transistor structure in a magnetic field in the quantum Hall regime. Using an illumination power of only 3 μW, our device generates a current of up to 400 nA without an applied bias, which corresponds to a photoresponsivity of 0.14 A/W. To the best of our knowledge, this is one of the highest values ever measured for single layer graphene. Furthermore, the high current suggests that every absorbed photon creates more than 8 charge carriers, so that carrier multiplication is apparent.

We discuss these photocurrents in the framework of magnetothermoelectric effects and recent calculations of photocurrent generation in edge channels [1]. Taking into account the observed gate voltage, magnetic field and polarization dependence, we develop a quasi-ballistic model for the measured photocurrent. It includes edge channel transport and charge carrier multiplication and is in good agreement with the experimental results.

[1] Queisser et al. Phys. Rev. Let. **111**, 046601 (2013)

TT 12.7 Mon 11:00 ER 270

Ballistic transport in graphene antidot arrays — •Andreas Sandner[1], Tobias Preis[1], Christian Schell[1], Paula Giudici[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

We report on the observation of antidot peaks in ρ_{xx} in monolayer-graphene (MLG), encapsulated between hexagonal boron nitride (hBN). The hBN-MLG-hBN heterostructures were fabricated with a dry transfer pick-up technique; subsequently mesas were etched in Hall bar geometry and contacted with 1-dimensional side contacts. The periodic antidot lattice was defined in a following step by additional electron-beam lithography and reactive ion etching.

We performed measurements on stacks with different antidot lattice periods down to 100 nm. Several peaks in magnetoresistance can be identified and assigned to orbits around one and several antidots. This proves ballistic transport in our graphene heterostructures, in spite of the critical etching step for small lattice periods. We show measurements at different temperatures and can study antidots peaks down to very low carrier densities ($n = 2 \cdot 10^{11}$ cm^{-2}) and magnetic fields ($B = 0.5$ T). At higher magnetic fields, well defined quantum Hall plateaus with filling factors down to $\nu = 1$ are observed, even at an antidot period of 100 nm.

TT 12.8 Mon 11:15 ER 270

Ballistic supercurrents in suspended graphene — •Markus Weiss and Christian Schönenberger — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel

Since the discovery of graphene there have been numerous efforts to use this material as a Josephson weak link between two superconductors. Devices based on oxidized silicon substrates have been produced a few years ago, and have shown bipolar, gate-tuneable supercurrents. The observation of effects are that unique to the Dirac semimetal graphene however has been prevented up to now by the large disorder modulation of the electric potential in graphene on silicon based substrates. For the direct observation of e. g. specular Andreev reflection, the disorder modulation of the Dirac point would have to be smaller that the proximity induced superconducting gap, a regime that cannot be reached in conventional devices. The road to cleaner graphene might go via deposition onto commensurate substrates like hexagonal boron nitride, or the removal of the silicon oxide substrate and suspension of graphene. The latter technique has been perfected in the recent years for devices with normal metal contacts, but turned out to be difficult to realize for superconducting contacts due to incompatibilities of superconducting materials with the fabrication process.

We have developed a device architecture that allows the realization of suspended graphene devices with superconducting contacts, and will show first experimental results, like the ballistic Josephson current through a graphene weak link.

TT 13: Focus Session: Functional Semiconductor Nanowires I (organized by HL)

The growth of nearly any kind of semiconductor in the form of nanowires as well as its properties have been intensely investigated in the past 15 years, because nanowires often offer superior properties compared to their bulk or thin-film counterparts. To fully exploit their unique properties, the challenging step is the integration of semiconductor nanowires into specific functional environments and devices. In this focus session, we present and offer a platform to discuss recent developments in exactly this area with applications in electronics, photonics and optoelectronics.

Organization: Carsten Ronning (FSU Jena), Martin Eickhoff (JLU Giessen), Tobias Voss (TU Braunschweig)

Time: Monday 9:30–13:15 Location: EW 201

Invited Talk TT 13.1 Mon 9:30 EW 201

Exploring the optical properties of 1D nanomaterials at sub-nanometer scale with a direct correlation to its structure at atomic scale — •Jordi Arbiol — Institució Catalana de Recerca i Estudis Avançats (ICREA), 08010 Barcelona, CAT, Spain — Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, E-08193 Bellaterra, CAT, Spain

Technology at the nanoscale has become one of the main challenges in science as new physical effects appear and can be modulated at will. New generations of functionalized materials are taking advantage of the low dimensionality, improving their properties and opening a new range of applications. As developments in materials science are pushing to the size limits of physics and chemistry, there is a critical need for understanding the origin of these unique physical properties (optical and electronic) and relate them to the changes originated at the atomic scale, e.g.: linked to changes in (electronic) structure of the material. Combining advanced electron microscopy imaging with electron spectroscopy, as well as cathodoluminescence in a STEM will allow us to probe the elemental composition and electronic structure simultaneously with the optical properties in unprecedented spatial detail. The

seminar will focus on several examples in advanced nanomaterials for optical and plasmonic applications. In this way the latest results obtained by my group on direct correlation between optical properties at sub-nanometer scale and structure at atomic scale will be presented.

TT 13.2 Mon 10:00 EW 201

Selective Area Growth of GaN Nanowires and Nanotubes — •Martin Hetzl[1], Fabian Schuster[1], Saskia Weiszer[1], Jose A. Garrido[1], María de la Mata[2], Jordi Arbiol[2], and Martin Stutzmann[1] — [1]Walter Schottky Institut and Physics Department, Technische Universität München, Garching, Germany — [2]Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Bellaterra, Spain

Selective area growth (SAG) of GaN nanowires (NWs) by molecular beam epitaxy has been investigated in a systematic way. A high uniformity of SAG NWs and a complete suppression of unintentional growth has been achieved. The nucleation sites were predefined by a titanium mask structured by e-beam lithography. The underlying growth kinetics will be addressed by varying the substrate temperature, the III/V-ratio, the growth time and the NW arrangement. For that, diamond (111) substrates have been used as a model material. However, successful transfer of SAG on Si (111), c-plane sapphire and other substrates confirms the general validity of the presented growth mechanism. Scanning transmission electron microscopy has been performed to investigate the structural quality of the NWs and to determine the polarity of the wurtzite lattice. At lower temperatures, so called "tripods" instead of NWs can occur, which result from large GaN zinc blende nuclei. The exact NW arrangement changes the local III/V-ratio. This has been used to force a transition from GaN NW to nanotube growth, leading to a much higher effective surface-to-volume ratio. The controllability of SAG GaN NWs represents an important step towards NW-based devices, e.g. for optoelectronics, sensing or catalysis.

TT 13.3 Mon 10:15 EW 201

Stability of heteroepitaxial coherent growth modes on nanowire radial surfaces — •Thomas Riedl[1,2] and Jörg Lindner[1,2] — [1]University of Paderborn, Department of Physics, Warburger Straße 100, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), Warburger Straße 100, 33098 Paderborn, Germany

Semiconductor nanowires (NWs) exhibit a large surface-to-volume ratio and are therefore interesting as a substrate for the growth of nanoscale heteroepitaxial islands as well as core-shell structures for use in optoelectronic applications. Compared to planar substrates the NW curvature leads to a modified thermodynamic stability of the coherent Frank-van-der-Merwe and Stranski-Krastanov (SK) heteroepitaxial growth modes. In the present contribution we investigate the stability of these growth modes on cylindrical NWs by means of continuum theory. In contrast to previous studies (i) the exact geometrical shape of pyramidal islands and (ii) the impact of the island contact angle on the elastic relaxation energy are considered. Maps of the growth mode stability are derived for the Si core / Ge shell structure, which display the favoured mode as a function of deposited volume, wetting layer thickness and NW radius. When using a Ge surface energy of 1.3 J/m^2 for both the shell and the pyramid surfaces the SK mode becomes stable only for large contact angles and NW radii larger than 40 nm. However, if the reduced surface energy of low-index Ge facets is taken into account, the transition between the two growth modes is shifted to smaller NW radii, as observed in experiments.

TT 13.4 Mon 10:30 EW 201

Cd_3As_2 Nanowires by Chemical Vapour Deposition — •Piet Schönherr and Thorsten Hesjedal — Department of Physics, Clarendon Laboratory, University of Oxford, Oxford OX1 3PU, United Kingdom

Cd_3As_2 has been well known for its very high mobility. Recently, it was discovered that the material displays two Dirac points with linearly dispersing states that are stabilized by crystal symmetry (three-dimensional Dirac semimetal). The Dirac cones live in three-dimensional k-space unlike topological insulators that only have two-dimensional Dirac cones on their surface. This makes Cd_3As_2 a three-dimensional analogue of graphene.

We present the growth and characterisation of Cd_3As_2 nanowires including results from electric transport measurements. Nanowires with a diameter as small as 10 nm were grown in a self-catalysed vapour-liquid-solid process using chemical vapour deposition. We analyse the growth mechanism and compare the vibrational modes of Cd_3As_2 nanostructures with bulk samples.

TT 13.5 Mon 10:45 EW 201

MOCVD Growth and Characterization of InGaN/GaN Nanowire-based core/shell Heterostructures — Bartosz Foltynski, Christoph Giesen, and •Michael Heuken — AIXTRON SE, Dornkaulstr. 2, 52134 Herzogenrath, Germany

GaN based nanostructures have stimulated great interest in their applications for fabricating next-generation light emitting diodes (LEDs) for solid state lighting (SSL). Nanowires, benefiting from their geometry and offer a set of extraordinary properties like increase of light emission by utilizing the nanostructure side walls, limitation of negative effect of polarization fields and reduction of dislocation density. In our studies we present the optical and structural characterization of InGaN/GaN core/shell nanowires grown on Si(111) substrates by MOCVD. SEM,Photoluminescence and cathodoluminescence were used as characterization techniques. All growth experiments were performed in an AIXTRON CCS (Close Coupled Showerhead) reactor. The self-organized GaN nanowires were grown on Si(111) substrates using AlN buffer and in-situ SiNx masking layer. The growth conditions were optimized to achieve maximum density of vertical GaN microrods perpendicularly aligned to the substrate. Detailed results on growth optimization and structure characterization will be presented and discussed.

TT 13.6 Mon 11:00 EW 201

Modulation doped GaAs-AlGaAs core-shell nanowires — •Dominik Irber[1], Stefanie Morkötter[1], Jonathan Becker[1], Nari Jeon[2], Daniel Rudolph[1], Bernhard Loitsch[1], Markus Döblinger[3], Max Bichler[1], Jonathan J. Finley[1], Lincoln J. Lauhon[2], Gerhard Abstreiter[1,4], and Gregor Koblmüller[1] — [1]Walter Schottky Institut and Physik Department, Technische Universität München, Garching, Germany — [2]Department of Materials Science and Engineering, Northwestern University, Evanston, U.S.A. — [3]Department of Chemistry, Ludwig-Maximilians-Universität München, Munich, Germany — [4]Institute for Advanced Study, Technische Universität München, Garching, Germany

In this work we will present electrical and structural properties of GaAs-AlGaAs core-shell nanowire (NW) MODFETs. The GaAs core was grown on Si (111) substrates via [111]-oriented self-catalyzed growth using MBE, followed by a Si δ-doped radial <110>-oriented AlGaAs shell. Using HRTEM and atom probe tomography (APT), the structure and elemental composition of the NWs were analyzed. The APT analysis revealed the position of the δ-doped layer and the Si dopant concentration, allowing to calculate the expected 2DEG carrier density. Electrical measurements using a top gate geometry verified the expected 2DEG density and further showed very steep switching behavior (SS=70mV/dec) with on/off-ratios $>10^4$ at 300K. The device geometry allowed to measure mobility at different sites of the NW. In combination with the APT data the influence of structural parameters on mobility can be studied.

Coffee break

Invited Talk TT 13.7 Mon 11:30 EW 201

Studying single semiconductor nanowires using a hard X-ray nanoprobe — •Gema Martinez-Criado — European Synchrotron Radiation Facility, Grenoble, France

Semiconductor nanowires present great advantages for optoelectronic and spintronic nanodevices. Their applications are basically controlled by multiple property-function relationships taking place at the nanoscale in the spatial and time regimes. Only a combination of high-resolution methods offer a comprehensive characterization of their complex nature. Here we present how a multimodal hard X-ray nanoprobe addresses fundamental questions in nanowire research. Selected topics ranging from cluster formation, dopant segregation, and phase separations to quantum confinement effects are examined with sub-100 nm spatial resolution and sub-50 ps temporal resolution. This scheme opens new opportunities for structural, composition and optical investigations with large potential in materials science.

TT 13.8 Mon 12:00 EW 201

Influence of surface depletion on electrical conductivity of freestnding GaAs nanowires investigated by a multi-tip STM — •Weihong Zhao[1], Matthias Steidl[1], Stefan Korte[2], Hubertus Junker[2], Werner Prost[3], Peter Kleinschmidt[1], and

Thomas Hannapel[1] — [1]Photovoltaics Group, Institute for Physics, Technische Universität Ilmenau, D-98684 Ilmenau — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, D-52425 — [3]CeNIDE and Center for Semiconductor Technology and Optoelectronics, University of Duisburg-Essen, D-47057 Duisburg

P-type Zn-doped GaAs-Nanowires were prepared by the Au-assisted vapor-liquid-solid growth mode in a metal-organic vapor phase apparatus. Electrical investigation was carried out by a multi-tip scanning tunneling microscope as nano-prober on free-standing p-GaAs nanowires. As an approach to understand the doping process through the growing process, Zn-doped GaAs nanowires with different diameter were prepared. The electrical measurements and analysis on the nanowires deliver the key-information about process related dopant incorporation along the nanowires, which is responsible for the varying charge carrier depletion thickness.

TT 13.9 Mon 12:15 EW 201

Antimony doped ZnO nanowires — •Thomas Kure[1], Alexander Franke[1], Sarah Schlichting[1], Emanuele Poliani[1], Felix Nippert[1], Markus R. Wagner[1], Marcus Müller[2], Peter Veit[2], Sebastian Metzner[2], Frank Bertram[2], Eswaran S. Kumar[3], Faezeh Mohammadbeigi[3], Jürgen Christen[2], Janina Maultzsch[1], Simon Watkins[3], and Axel Hoffmann[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Otto-von-Guericke-University, Institut für Experimentalphysik, Germany — [3]Simon Fraser University, Department of Physics, Burnaby, Canada

We investigated the morphology of metalorganic vapor phase epitaxy (MOVPE) grown c-axis aligned Sb doped ZnO NWs as well as the doping distribution and structural defects of single NWs. Cathodoluminescence spectroscopy (CL) along several single NWs reveal that the luminescence stems predominately from the tip and decreases towards the bottom of the NW. Raman measurements on ensemble NWs show additional vibrational modes, where some appear exclusively in Sb doped ZnO. Tip-enhanced Raman spectroscopy (TERS) was performed to investigate the local doping concentration. The significant increase of Sb-related Raman modes towards the apex confirms the increase of Sb along the NW.

TT 13.10 Mon 12:30 EW 201

Hard X-ray detection in a single 100 nm-diameter nanowire — •Jesper Wallentin[1], Markus Osterhoff[1], Robin Wilke[1], Karl-Magnus Persson[2], Lars-Erik Wernersson[2], Michael Sprung[3], and Tim Salditt[1] — [1]Institute for X-Ray Physics, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Department of Electrical and Information Technologies, Lund University, Lund S-221 00, Sweden — [3]DESY, Notkestrasse 85, 22607 Hamburg, Germany

While hard X-rays can now be focused below 10 nm, current semiconductor-based X-ray detectors have pixel sizes of tens of micron. It is desirable to shrink the detector pixel size in order to improve the resolution in imaging, spectroscopy and crystallography, but smaller detector volumes are expected to lead to a weak electrical signal. We investigated the electrical response of a 100 nm-diameter InP nanowire exposed to a hard X-ray nanofocus. A fixed bias voltage was used, and the current was measured with a picoammeter. The conductance increased about 4 orders of magnitude under full X-ray flux. Dynamic measurements revealed very slow processes, with lifetimes at the order of seconds. Such long lifetimes, possibly related to surface states, could explain the strong X-ray induced current. As a demonstration of the potential of nanowires as X-ray detectors, we imaged the X-ray nanofocus by making a 2D raster with the device. The spatial resolution was less than 1 micron, and could be improved by making devices with the nanowire oriented along the optical axis. These results show that nanostructures can have much stronger X-ray response than expected from a simple scaling of bulk parameters.

TT 13.11 Mon 12:45 EW 201

synchrotron X-ray photoelectron spectroscopy study of GaAs/InAs core/shell nanowires grown by MBE — •Behnam Khanbabaee[1], Torsten Rieger[2], Nataliya Demarina[2], Detlev Grützmacher[2], Mihail Ion Lepsa[2], Rainer Timm[3], and Ullrich Pietsch[1] — [1]Solid State Physics, Dept. of Physics, University of Siegen, Siegen, Germany — [2]Peter Grünberg Institute and JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany — [3]Synchrotron Radiation Research and The Nanometer Structure Consortium, Dept. of Physics, Lund University, Lund, Sweden

Semiconductor nanowire (NW) heterostructures are promising building blocks for future electronic devices. In particular, GaAs/InAs radial NWs heterostructures are candidates for nano-electronics, where a lower band gap semiconductor, e.g. InAs, is grown on a semiconductor with a higher band gap, e.g. GaAs, providing band bending at the interface. For effective band confinement it is necessary to control the radial thickness, and the local defect structure at the hetero-interface and its relation to the electronic properties. Here we report on X-ray photoelectron spectroscopy of GaAs/InAs core/shell NWs grown by molecular beam epitaxy. After cleaning under atomic hydrogen the As-oxides on top of the NWs were considerably reduced while the Ga- and In-oxides were slightly reduced. The binding energy of the As 3d core levels was shifted about 1 eV towards lower energies. These results show that the As component of the native oxide turns the NWs surface strongly n-type. Our findings show that the shelling of GaAs NWs with InAs may leads to band bending of 0.2 to 0.3 eV at hetero-interface.

TT 13.12 Mon 13:00 EW 201

Seebeck effect measurements on single InAs and GaAs nanowires — •Alexander Hirler[1], Vanessa Schaller[1], Jonathan Becker[1], Bernhard Loitsch[1], Stefanie Morkötter[1], Julian Treu[1], Gerhard Abstreiter[1,2], Jonathan Finley[1], and Gregor Koblmüller[1] — [1]Walter Schottky Institut and Physik Department, TU München, Garching, Germany — [2]TUM Institute of Advanced Study, Garching, Germany

We present recent results on measurements of the Seebeck coefficient of intrinsic n-type InAs and carbon doped p-type GaAs nanowires (NWs) grown on Si(111) substrates via catalyst free molecular beam epitaxy. To measure the Seebeck effect on single NWs, a temperature gradient is applied via lithographically fabricated heating coils and measured by two resistance thermometers each in a four-point measurement geometry, which also act as electric contacts to the NW. Equipped with another heating resistor the temperature dependent Seebeck-coefficient can be measured as well. Compared to field effect transistor (FET) measurements, the carrier density can be conducted independent of the gate geometry. In addition, the carrier type can be determined from the sign of the Seebeck voltage. Seebeck measurements presented here, demonstrate successful p-type doping of GaAs NWs via carbon. P-type doping and the quantitative measurement of the doping concentration via Seebeck measurements are important steps towards future heterojunction NW devices.

TT 14: Surface Magnetism – Skyrmions (jointly with MA, O)

Time: Monday 9:30–12:45 Location: EB 301

TT 14.1 Mon 9:30 EB 301

Dynamics of spin spirals and skyrmions in temperature gradient — •Rocio Yanes, Denise Hinzke, and Ulrich Novak — Universität Konstanz, Konstanz, Germany

Recently, Dzyaloshinskii-Moriya (DM) interaction has attracted attention in magnetism since it can lead to the formation of skyrmions and spin spirals with promising applications in spintronics [1,2]. Furthermore, it has been shown that temperature gradients can cause magnonic spin currents and with that spin transfer torques leading to a movement of a domain wall in a magnetic nanowire [3,4]. In this work, we combined both topics to analyze the dynamics of two dimensional non-collinear magnetic textures subject to a temperature gradient.

Numerical calculations of the dynamics of helical spin spiral (HSS), skyrmion lattices and isolated skyrmions are carried out for different values of the temperature gradient and damping parameter. Our results show that the HSS moves towards the hotter area driven by the temperature gradient. The velocity of this movement is asymmetric with respect to the sign of the temperature gradient due to the effect of the DM interactions. We observe a clear difference between the movement of isolated skyrmions and skyrmion lattices. While in the first case, the skyrmion motion is determine by the temperature gradient and the Magnus force, in the case of a lattice of skyrmions the interaction between skyrmions plays a fundamental role.

[1] A. Fert et al. Nature Nanotech., 8, 152, (2013). [2] N. Nogoasa et al., Nature Nanotech., 8, 899 (2013). [3] D. Hinzke and U. Novak, PRL, 107, 027205 (2011). [4] Schlickeiser et al., PRL, 113, 097201 (2014).

TT 14.2 Mon 9:45 EB 301

Interlayer Exchange Coupling: A route to stabilize skyrmions in magnetic multilayers — •Ashis K. Nandy, Nikolai S. Kiselev, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Magnetic skyrmion is a topologically nontrivial spin texture with particle like properties, which may emerge quite generally under an applied magnetic field of appropriate strength in any magnetic thin layer or multilayer with surface or interface induced Dzyaloshinskii-Moriya interaction (DMI). DMI chooses chirality i.e. the proper sense of rotation of spins [1]. However, the required magnetic field to stabilize skyrmions can be excessively large. We present a multiscale approach based on DFT calculations and atomistic spin-dynamic simulations, which allows us to stabilize skyrmions in magnetic multilayers even at zero magnetic field. It is based on fine tuning the interplay between internal and interfaces induced interactions by adjusting the thicknesses and interface compositions of multilayers. Our approach predicts the existence of a skyrmion lattice as well as isolated skyrmions in a thin film of a transition-metal monolayer grown on a heavy metal substrate. The simulated skyrmions exhibit high stability in an applied magnetic field and temperature. We provide a description for the complex phases occurring in such systems and present a magnetic phase diagram for a prototype example of Mn/W(001).

[1] M. Bode *et al.*, Nature **447**, 190 (2007).

TT 14.3 Mon 10:00 EB 301

Observation of spin transfer torques in the transverse magnetic susceptiblity of the Skyrmion lattice phase of MnSi — •Felix Rucker, Christoph Schnarr, Andreas Bauer, Alfonso Chacon, Philipp Köhler, and Christian Pfleiderer — Lehrstuhl für Topologie korrelierter Systeme, Technische Universität München, Garching, Germany

In the skyrmion lattice phase of MnSi the observation of sizeable spin transfer torques [1-3] in small angle neutron scattering and the Hall resistivity for current densities already five orders of magnitude smaller as compared to conventional magnetic materials promises easy experimental access to the precise qualitative and quantitative form of the Landau Lifshitz Gilbert equation. We report measurements of the transverse magnetic susceptibility, $\chi_\perp$, in the skyrmion lattice phase of MnSi. As our main result we find a distinct increase of $\chi_\perp$ with increasing current density around the critical current density j_c. We discuss the broader implications of our experimental findings, which provide, for the first time, a direct link between a thermodynamic property and the effects of spin transfer torques in skyrmion lattices.

[1] F. Jonietz et al., Science **330**, 1648 (2010)
[2] T. Schulz et al., Nat. Phys. **8**, 301 (2012)
[3] K. Everschor et al., Phys. Rev. B **86**, 054432 (2012)

TT 14.4 Mon 10:15 EB 301

Magnetic skyrmions stabilized at zero field — •Nikolai S. Kiselev[1], Ashis K. Nandy[1], Changhoon Heo[2], Theo Rathing[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Molecules and Materials, Radboud University Nijmegen, 6525 AJ Nijmegen, Netherlands

Magnetic skyrmions may appear as a metastable state in thin magnetic layers at zero magnetic field within certain range of Dzyaloshinskii-Moriya interaction and the uniaxial anisotropy. We present a comprehensive theoretical study of the statics and dynamics of such skyrmions. Important feature of this solution is a coexistence of two type of skyrmion solutions characterized by opposite polarity and opposite topological charge. We consider such skyrmions as a conceptually new approaches in data storage where switching between two of such skyrmion states is provided by sort magnetic field pulse. We discuss complex mechanism of such switching. The role of field pulse duration, damping, size and shape of host system are discussed in details. Our results are based on stochastic spin dynamics simulation applied to an extended Heisenberg model for different type of crystal lattices.

TT 14.5 Mon 10:30 EB 301

Emergent electrodynamics in $Mn_{1-x}Fe_xSi$ — •Christoph Schnarr, Felix Rucker, Christian Franz, Robert Ritz, Andreas Bauer, and Christian Pfleiderer — Lehrstuhl für Topologie korrelierter Systeme, Technische Universität München, Garching, Germany

The emergent electrodynamics of the skyrmion lattice phase in chiral magnets comprise of an emergent magnetic field of one flux quantum per skyrmion that gives rise to an emergent electric field, when the skyrmion lattice moves under the application of spin currents exceeding a critical current density j_c [1,2]. We report a study of the emergent electrodynamics in $Mn_{1-x}Fe_xSi$, where we exploit a well understood increase of the topological Hall resistivity by an order of magnitude with increasing Fe concentration [3]. On the one hand, this allows us to track j_c for increasing emergent magnetic field in the presence of increasing disorder. On the other hand, we observe evidence for emergent electric fields even in the magnetoresistance, reflecting, in combination with the emergent electric field in the Hall signal, the direction of motion of the skyrmion lattice.

[1] F. Jonietz et al., Science **330**, 6011, 1648-1651 (2010)
[2] T. Schulz et al., Nature Physics **8**, 4, 301-304 (2012)
[3] C. Franz et al., Physical review letters **112**, 18, 186601 (2014)

15 min. break

TT 14.6 Mon 11:00 EB 301

Advanced characterization of helical spin structures and domains in Skyrmion systems — •Peggy Schönherr[1], Antoine Dussaux[1], Naoya Kanazawa[2], Yoshinori Tokura[2], Christian Degen[1], Manfred Fiebig[1], and Dennis Meier[1] — [1]ETH Zürich, 8093 Zürich, Switzerland — [2]University of Tokyo, 113-8656 Tokyo, Japan

Magnetic whirls, so-called Skyrmions, emerge in various chiral magnets and attract tremendous attention due to their exotic properties. Skyrmions can, e.g., be moved at ultra-low current densities and give rise to the topological Hall Effect. Much less is known about the magnetic phases that surround the Skyrmion state, including fundamental aspects such as the domain formation and spin-defect interactions. The fragmented knowledge is partially due to the challenging experimental access and the general difficulty to image antiferromagnetic order at the nanoscale. Here, we show how helical magnetic structures in the Skyrmion system FeGe emerge and transform as a function of temperature and magnetic field. We discuss the magnetic field-driven response of multi-domain states, the influence of defects, as well as fingerprints

of spontaneous jump-like movements of the periodic spin arrangement. The results are gained near room temperature using magnetic force microscopy (MFM) and diamond nitrogen-vacancy center microscopy. Besides providing new insight to the physics of Skyrmion materials, our results foreshadow a promising pathway for measuring complex spin textures with high spatial and temporal resolution.

TT 14.7 Mon 11:15 EB 301

Field-dependent Size and Shape of Single Magnetic Skyrmions — •Niklas Romming, André Kubetzka, Christian Hanneken, Kirsten von Bergmann, and Roland Wiesendanger — Department of Physics, University of Hamburg, 20355 Hamburg, Germany

Skyrmions are spatially localised solitonic magnetic whirls with axial symmetry and fixed rotational sense. They have recently been observed in both non-centrosymmetric bulk crystals and in ultrathin transition metal films on heavy-element substrates as a result of sizable Dzyaloshinskii-Moriya interactions. In addition to their protected topology and nano-scale size, skyrmions can easily be moved by lateral spin currents and written as well as deleted by vertical spin-current injection. Here we use spin-polarised scanning tunnelling microscopy to directly reveal the field-dependent internal spin structure of individual skyrmions in a biatomic PdFe layer on Ir(111) [1] with atomic-scale precision. An analytical expression for the description of skyrmions is proposed, which can establish a connection between the original work - predicting magnetic skyrmions - and their experimentally determined magnetic-field dependent size and shape. Thus, the relevant material parameters responsible for skyrmion formation can be determined. [1] N. Romming et al., Science 341, 636 (2013).

TT 14.8 Mon 11:30 EB 301

Spin dynamics of spin-orbit coupled dimers on Pt(111) — •Manuel dos Santos Dias and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

The interaction between two magnetic adatoms becomes anisotropic in the presence of strong spin-orbit coupling (SOC). The broken inversion symmetry at the surface leads in particular to the Dzyaloshinksii-Moriya interaction, enabling chiral magnetic ground states. We study the impact of this interaction on the spin dynamics of magnetic dimers (e.g. Fe) on the Pt(111) surface, in connection to possible inelastic scanning tunneling spectroscopy (ISTS) experiments [1]. We employ our recently developed time-dependent density functional theory including SOC, based on the Korringa-Kohn-Rostoker Green function approach. An extension of our theoretical ISTS method [2] to incorporate SOC is in progress.

Work funded by the HGF-YIG Programme FunSiLab - Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] A. A. Khajetoorians et al., Phys. Rev. Lett. **111**, 157204 (2013)
[2] B. Schweflinghaus et al., Phys. Rev. B **89**, 235439 (2014)

TT 14.9 Mon 11:45 EB 301

First-principles study of confined magnetic skyrmions in Pd/Fe/Ir(111) — •Dax Michael Crum[1,2], Benedikt Schweflinghaus[1], Mohammed Bouhassoune[1], Juba Bouaziz[1], Stefan Blügel[1], and Samir Lounis[1] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Microelectronics Research Center, The University of Texas at Austin, Austin Texas, 78758 USA

We investigate for the first time confined skyrmionic magnetic defects in an otherwise ferromagnetic thin film from first-principles. The system of choice is Pd/Fe on Ir(111) [1,2]. Utilizing the full-potential relativistic Korringa-Kohn-Rostoker Green functions formalism, we investigate in real-space the energetics of creating single chiral magnetic textures purely from *ab initio*. We find that the nano-skyrmion structures become energetically more favorable with increasing size. We interpret the results by extracting the tensors of magnetic exchange interactions and modeling the system within an extended Heisenberg Hamiltonian, where the Dzyaloshinskii-Moriya interaction plays a key role. We also investigate the theoretical scanning tunneling microscopy spectra by analysing the local density of states in vacuum near the skyrmion surface and make connection to available experiments [1].

This work is supported by the HGF-YIG Programme VH-NG-717 (Functional Nanoscale Structure and Probe Simulation Laboratory – Funsilab) and the US National Science Foundation (NSF).
[1] Romming *et al.*, Science **341**, 636 (2013).
[2] B. Dupé *et al.*, Nature Communications **5**, 4030 (2014).

TT 14.10 Mon 12:00 EB 301

Energy-dependent magnetic contrast of a nanoscale spin helix measured by STM — •Safia Ouazi, Soo-Hyon Phark, Jeison A. Fischer, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

Helical spin order has been revealed for Fe bilayer islands on Cu(111) by spin-polarized scanning tunneling spectroscopy (SP-STS) in a magnetic field at 10 K [1]. We measure the magnetic contrast, as given by the difference in differential conductance for states with and without spin helix [1], as a function of the gap voltage applied between tip and sample. Thus, we obtain the first spatially- and energy-resolved map of spin contrast for a nanoscale spin spiral. The wave vector describing the helical spin order remains constant in the energy range -0.8eV to +0.5eV, whereas the spin contrast shows a strong modulation. This result identifies a novel aspect of SP-STM to characterize complex spin order with respect to the corresponding electronic band structure. We discuss the results in view of a partial energy gap associated with the non-collinear spin order.

[1] S.-H. Phark, J.A. Fischer, M. Corbetta, D. Sander, K. Nakamura, J. Kirschner, Nat. Commun. 5:5183 doi:10.1038/ncomms6183 (2014).

TT 14.11 Mon 12:15 EB 301

A Magnetic Nano-Skyrmion Lattice observed in a Si-wafer based Multilayer System — •Stefan Krause[1], Anika Schlenhoff[1], Philipp Lindner[1], Johannes Friedlein[1], Roland Wiesendanger[1], Michael Weinl[2], Matthias Schreck[2], and Manfred Albrecht[2] — [1]Department of Physics, University of Hamburg, Germany — [2]Institute of Physics, University of Augsburg, Germany

Recently, an atomic-scale two-dimensional magnetic skyrmion lattice at the Fe/Ir(111) interface has been discovered using spin-polarized scanning tunneling microscopy (SP-STM).[1] Skyrmions offer new exciting possibilities for spintronic applications, using them as digital information carriers. For these applications the mass production of devices using multilayer growth on large-scale substrates is indispensable.

In 2009, the heteroepitaxial growth of single crystal Ir(111) films on Si(111) wafers with yttria-stabilized zirconia buffer layers has been demonstrated.[2] For our study we epitaxially grow one monolayer of Fe on top of this multilayer substrate. The SP-STM experiments reveal a magnetic skyrmion lattice, being fully equivalent to the magnetic ground state that has previously been observed on an Ir(111) bulk single crystal substrate. In addition, it is found to be robust against local atomic lattice distortions induced by multilayer preparation. Our work paves the way towards spintronic applications of nano-skyrmions in ultrathin films and multilayer systems.

[1] S. Heinze *et al.*, Nature Physics **7**, 713 (2011).
[2] S. Gsell *et al.*, J. Cryst. Growth **311**, 3731 (2009).

TT 14.12 Mon 12:30 EB 301

Tailoring a Spin Spiral by Uniaxial Strain — •Pin-Jui Hsu, Aurore Finco, Lorenz Schmidt, Andre Kubetzka, Kirsten von Bergmann, and Roland Wiesendanger — Department of Physics, Hamburg Univerisyt, 20355 Hamburg, Germany

Spin spirals typically result from competing magnetic interactions. In the presence of a sizable Dzyaloshinskii-Moriya (DM) interaction, the spin spirals exhibit a unique rotational sense and their periodicity is governed by the ratio of the exchange and DM-interaction strength. Spin-polarized scanning tunneling microscopy (SP-STM) experiments have already revealed several examples of cycloidal and conical spin spiral states in ultrathin films of magnetic transition metals (e.g. Fe, Mn, Cr) on heavy-element substrates (e.g. W, Ir). Here, we report on a SP-STM study on two monolayers of Fe on Ir(111) where a regular dislocation line structure with a periodicity of 3.71 ± 0.47 nm is observed due to the strain relief of bcc(110) Fe grown epitaxially on the Ir(111) substrate. SP-STM reveals the presence of cycloidal spin spirals with a period of 1.82 ± 0.15 nm which are guided by the dislocation lines to form a well-defined spin-ordered state. These ordered spin spirals form an undulating pattern perpendicular to the dislocation lines wiggling with an angle of about 155^o, indicating an interaction between structural relaxation and the observed spin structure, particularly along the three symmetrically equivalent crystallographic axes. In contrast, a disordered spin spiral state, which locally exhibits a period of 1.38 ± 0.22 nm is observed in the regions without dislocation lines.

TT 15: Focus Session: Skyrmionics: Future of Spintronics? (jointly with MA)

Major challenges faced by the spintronics community concern the stability and speed of processing information and the packing density of data stored. Present day limitations in spintronics may be traced to the use of conventional magnetic materials and how these materials are tailored to meet advanced technological requirements. The recent discovery of topological spin soliton lattices, frequently referred to as skyrmion lattices in recognition of seminal field-theoretical contributions of British nuclear physicist Toni Skyrme, as well as the possibility to generate isolated skyrmions as generic magnetic properties of bulk compounds, thin films, interfaces and surfaces has revealed several remarkable properties. These comprise of greatly enhanced stability due to their non-trivial topological winding, new capabilities to create and destroy magnetically encoded information, efficient coupling to spin currents generating spin transfer torques at dramatically reduced current densities, and last but not least, the capability to purpose-design broad-band spin dynamics devices.

This Focus Session aims to review critically the status of experimental and theoretical studies on skyrmions in non-centrosymmetric compounds and interface-driven spin-systems in the context of their potential for spintronics applications.

Organizers: Christian Back (Uni Regensburg) and Christian Pfleiderer (TU München)

Time: Monday 15:00–17:45 Location: H 0104

Invited Talk TT 15.1 Mon 15:00 H 0104
Skyrmion Dynamics — •Yoshinori Tokura — RIKEN Center for Emergent Matter Science, Wako, Japan — University of Toyo, Tokyo, Japan

Dynamics of skyrmions have been investigated in terms of real-space observation by Lorentz transmission microscopy, topological transport phenomena, and micromagnetic simulations. Key functions toward 'skyrmionics' are discussed.

Topical Talk TT 15.2 Mon 15:30 H 0104
Topological Transport Phenomena in Magnetic Skyrmion Matter — •Markus Garst — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

Magnetic skyrmions are topological textures with a finite winding number – similar to the baryon number in nuclear matter – which is at the origin of various novel transport phenomena. It is directly reflected in a strong spin-Magnus force in their effective equation of motion resulting in a peculiar dynamics with skyrmions preferentially moving along equipotential lines akin to guiding centers of electrons in Landau levels. This not only allows for an efficient manipulation by spin currents but also enables skyrmions to avoid pinning centers giving rise to spintronic phenomena at ultralow threshold currents [1]. Moreover, the adiabatic motion of electrons in skyrmion textures results in an emergent electrodynamics revealed by a topological Hall effect and a skyrmion-flow Hall effect [2]. Interesting spin-thermal transport and skyrmion caloritronic phenomena are also to be expected in insulators. The topological winding number is manifest in the magnon-skyrmion scattering potential and, for example, leads to magnon skew scattering and a magnon Hall effect. In turn, the magnon pressure generated, e.g., by a thermal gradient induces, counterintuitively, a skyrmion motion towards the hot region, i.e., the magnon source [3].

[1] F. Jonietz *et al.*, Science **330**, 1648 (2010)
[2] T. Schulz *et al.*, Nat. Phys. **8**, 301 (2012)
[3] C. Schütte and M. Garst, Phys. Rev. B **90**, 094423 (2014)

Invited Talk TT 15.3 Mon 16:00 H 0104
Interface Induced Individual Skyrmions in Thin Films and Multilayers — K. Bouzehouane[1], V. Cros[1], C. Deranlot[1], •A. Fert[1], K. Garcia[1], C. Moreau-Luchaire[1], N. Reyren[1], J.-M. Sampaio[1,3], N. van Horne[1], M. Chshiev[2], Hongxin Yang[2], A. Thiaville[3], S. Rohart[4], C. Moutafis[4], C.A.F. Vaz[4], P. Warnicke[4], J. Raabe[4], and M. Weigand[5] — [1]Unité Mixte de Physique CNRS/Thales, 1 Av. Fresnel, 9767 Palaiseau, France — [2]Université de Grenoble, and SPINTEC (CNRS/CEA-INAC), 38054 Grenoble Cedex, France — [3]Laboratoire de Physique des Solides, Université Paris-Sud, CNRS-UMR 8502, 91405 Orsay Cedex, France — [4]Swiss Light Source, Paul Scherrer Institute, 5232 Villigen, Switzerland — [5]Max Planck Institute for Intelligent Systems, Heisenbergstraße 3, 70569 Stuttgart, Germany

This talk is on individual skyrmions induced by interface Dzyaloshinskii-Moriya Interactions (DMI) in thin magnetic films or multilayers. I will present:

(1) Ab-initio calculations clearing up characteristic features of interface DMI: extension of the DMI away from the interface spins and thickness dependence, influence of the existence of proximity-induced magnetism in the spin-orbit layer, influence of interface roughness.

(2) Micromagnetic simulations of the nucleation and current-induced motion of skyrmions.

(3) Preliminary experimental results on (Ir/Co/Pt)x10 multilayers.

15 min. break.

Topical Talk TT 15.4 Mon 16:45 H 0104
Magnetic Skyrmions and Chiral Spin Structures in Ultra-Thin Films — •Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Ultrathin magnetic films and heterostructures provide a fantastic playground for the stabilization, manipulation and usage of magnetic skyrmions – topological magnetization solitons – magnetic entities with particle like properties that may open a new vista for spintronics. A crucial quantity for the skyrmion formation is the Dzyaloshinskii-Moriya interaction (DMI), whose presence in thin films could be established in a concerted effort of first-principles theory and spin-polarized scanning tunneling microscopy [1]. It could be shown that the spin-orbit interaction and the structure inversion-asymmetry in these systems result in a DMI that is strong enough to give rise to one-dimensional and two-dimensional lattices [2] of chiral spin-textures as well as chiral domain walls. Even single skyrmions [3] could be induced. In retrospect, it is surprising how little is known about the DMI in these metallic systems. In this talk I give some insight into the DMI, the relation to the transport properties of electrons such as the THE and AHE in connection to the spin texture of a skyrmion, and discuss possibilities to manipulate the magnetic interaction to enlarge the materials base to stabilize single skyrmions.

[1] M. Bode *et al.*, Nature **447**, 190 (2007)
[2] S. Heinze *et al.*, Nature Phys. **7**, 713 (2011)
[3] N. Romming *et al.*, Science **341**, 636 (2013)

Invited Talk TT 15.5 Mon 17:15 H 0104
Racetrack Memory: Highly Efficient Current Induced Domain Wall Motion in Synthetic Antiferromagnetic Racetracks — •Stuart Parkin — Max Planck Institute for Microstructure Physics, Halle, Germany — IBM Research - Almaden, San Jose, California, USA

Memory-storage devices based on the current controlled motion of domain walls in magnetic racetracks promise performance and reliability beyond that of conventional magnetic disk drives and solid state storage devices. Racetracks that are formed from atomically thin, perpendicularly magnetized nano-wires, interfaced with adjacent metal layers with high spin-orbit coupling, give rise to domain walls possessing a chiral Néel structure. These domain walls can be moved very efficiently with current. However, high capacity racetrack memory

requires closely-packed domain walls whose density is limited by dipolar coupling from their fringing magnetic fields. These fields can be eliminated using a spin-engineered synthetic antiferromagnetic (SAF) structure composed of two magnetic sub-layers, exchange-coupled via an ultrathin antiferromagnetic-coupling spacer layer. We show that nano-second long current pulses can move domain walls in SAF racetracks that have nearly no net magnetization. Surprisingly, we find that the domain walls can be moved even more efficiently and at much higher speeds of up to $\sim$ 750 m/sec compared to similar racetracks in which the sub-layers are coupled ferromagnetically. The origin of these giant current induced domain wall velocities is discussed.

TT 16: Transport: Quantum Coherence and Quantum Information Systems – Experiments (jointly with HL, MA)

Time: Monday 15:00–17:15 Location: H 0110

TT 16.1 Mon 15:00 H 0110

Coplanar microwave resonators for superconductor/cold atom hybrid devices — •Daniel Bothner, Dominik Wiedmaier, Benedikt Ferdinand, Martin Knufinke, Helge Hattermann, Patrizia Weiss, József Fortágh, Dieter Koelle, and Reinhold Kleiner — Physikalisches Institut and Center for Collective Quantum Phenomena in LISA$^+$, University of Tübingen, Germany

Recently, it has been demonstrated that ultracold atomic clouds can show very long coherence times on the order of 10 sec in close proximity to a superconducting chip surface [1]. Due to these extraordinarily long coherence times, atomic clouds are promising candidates as long-lived quantum memory in a future hybrid quantum processor. The realization of such a fully functioning hybrid system, however, poses severe challenges regarding the design and optimization of the superconducting chip. We will briefly discuss the relevant experimental boundary conditions and present strategies to comply with them on the way towards coherent coupling between ultracold atomic ensembles and on-chip microwave resonators. We in particular focus on how mixing normal conducting and superconducting components can outperform purely superconducting chips with respect to the requirements of the aspired hybrid system.

[1] S. Bernon *et al.*, Nature Commun. **4**, 2380 (2013)

TT 16.2 Mon 15:15 H 0110

Circuit QED with a gradiometric tunable-gap flux qubit — •Frank Deppe[1,2,3], Manuel J. Schwarz[1,2,3], Max Haeberlein[1,2,3], Jan Goetz[1,2,3], Alexander Baust[1,2,3], Peter Eder[1,2,3], Friedrich Wulschner[1,2,3], Edwar Xie[1,2,3], Ling Zhong[1,2,3], Kirill Fedorov[1,2,3], Edwin P. Menzel[1,2,3], Achim Marx[1,2,3], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

In circuit quantum electrodynamics or quantum simulation experiments, superconducting quantum bits must combine good coherence with high in situ tunability. Often, a large anharmonicity is also desirable. Other than the popular transmon, the gradiometric tunable-gap flux qubit meets all three of these requirements. Here, we fabricate and characterize such a qubit and demonstrate its first implementation into a transmission line resonator. We show spectroscopy and first time domain results.

This work is supported by the DFG via SFB 631 and the EU projects CCQED and PROMISCE.

TT 16.3 Mon 15:30 H 0110

Flux qubit to a transmission line — •Max Haeberlein[1,2,3], Gustav Anderson[1,2], Lujun Wang[1,2], Alexander Baust[1,2,3], Peter Eder[1,2], Michael Fischer[1,2], Jan Goetz[1,2], Edwar Xie[1,2], Manuel Schwarz[1,2], Karl Friedrich Wulschner[1,2], Ling Zhong[1,2,3], Frank Deppe[1,2], Kirill Fedorov[1,2], Hans Hübl[1,2], Achim Marx[1], Edwin Menzel[1,2], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 München, Germany

Within the last decade, superconducting qubits coupled to microwave resonators have been extensively studied within the framework of quantum electrodynamics. Ultimately, quantum computing seems within reach in such architectures. However, error correction schemes are necessary to achieve the required fidelity in multi-qubit operations, drastically increasing the number of qubits involved.

In this work, we couple a flux qubit to a transmission line where it interacts with itinerant microwave photons granting access to all-optical quantum computing. In this approach, travelling photons generate entanglement between two waveguides, containing the qubit information.

In this presentation, we show experimental data on flux qubits coupled to transmission lines. Furhtermore, we will discuss entanglement generation between two separate paths.

This work is supported by the DFG via SFB 631 and EU projects CCQED and PROMISCE.

TT 16.4 Mon 15:45 H 0110

Ultrastrong coupling of a flux qubit — •A. Baust[1,2,3], E. Hoffmann[1,2,3], M. Haeberlein[1,2,3], M. J. Schwarz[1,2,3], P. Eder[1,2,3], J. Goetz[1,2,3], F. Wulschner[1,2,3], E. Xie[1,2,3], L. Zhong[1,2,3], K. G. Fedorov[1,2,3], E. P. Menzel[1,2,3], F. Deppe[1,2,3], A. Marx[1,2,3], and R. Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

Circuit quantum electrodynamics has not only become a versatile toolbox for quantum information processing, but is also a powerful platform for the investigation of light-matter interaction. The coupling strength between microwave resonators and qubits acting as artificial atoms can be tuned over several orders of magnitude and can even reach the regime of ultrastrong coupling. We present spectroscopic data of a flux qubit coupled galvanically to the signal lines of two coplanar stripline resonators. We discuss the complex mode spectrum and show that the coupling strength between the qubit and one resonant mode reaches 17% of the respective mode frequency. Noticably, the high coupling strength is reached solely by the geometric layout of the qubit without utilizing additional coupling elements such as Josephson junctions. Our data exhibit a pronounced Bloch-Siegert shift and therefore represent an experimental evidence for the breakdown of the Jaynes-Cummings model.

This work is supported by the DFG via SFB 631 and EU projects CCQED and PROMISCE.

TT 16.5 Mon 16:00 H 0110

Characterization of superconducting transmission line resonators — •Jan Goetz[1,2], Philipp Summer[1,2], Sebastian Meier[1,2], Marta Krawczyk[1], Max Häberlein[1,2], Alexander Baust[1,2,3], Karl Friedrich Wulschner[1,2], Edwar Xie[1,2,3], Peter Eder[1,2], Michael Fischer[1,2], Manuel Schwarz[1,2], Ling Zhong[1,2,3], Frank Deppe[1,2], Kirill Fedorov[1,2], Hans Hübl[1,2], Achim Marx[1], Edwin Menzel[1,2], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

Superconducting transmission line resonators are widely used in circuit quantum electrodynamics experiments as quantum bus or storage devices. For these applications, long coherence times, which can be linked to the internal quality factor of the resonators, are crucial. Here, we show a systematic study of the internal quality factor of niobium thin film resonators. We analyze different cleaning methods and substrate parameters for coplanar waveguide as well as microstrip geometries. In addition, we investigate the impact of a niobium-aluminum interface which is necessary for galvanically coupled flux qubits made from aluminum. This interface can be avoided by fabricating the complete resonator-qubit structure using $Al/AlO_x/Al$ technology during fabrication.

This work is supported by the DFG via SFB 631 and EU projects CCQED and PROMISCE.

TT 16.6 Mon 16:15 H 0110

Superconducting on-chip microwave interferometers — •Edwin P. Menzel[1,2,3], Michael Fischer[1,2,3], Christian Schneider[1,2,3], Alexander Baust[1,2,3], Peter Eder[1,2,3], Jan Goetz[1,2,3], Max Haeberlein[1,2,3], Manuel Schwarz[1,2,3], Karl Friedrich Wulschner[1,2,3], Edwar Xie[1,2,3], Ling Zhong[1,2,3], Frank Deppe[1,2,3], Kirill Fedorov[1,2,3], Hans Huebl[1,2,3], Achim Marx[1,2,3], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

In the realm of all-microwave quantum computation, information is encoded in itinerant microwave photons propagating along transmission lines. In such a system unitary operations are implemented by linear elements such as beam splitters or interferometers. However, for two-qubit operations non-linear gates, e.g., c-phase gates are required. In this work, we investigate superconducting interferometers as a building block of a c-phase gate. We experimentally characterize their scattering properties and compare them to simulation results. Finally, we discuss our progress towards the realization of a c-phase gate.

This work is supported by the DFG via SFB 631 and the EU projects CCQED and PROMISCE.

TT 16.7 Mon 16:30 H 0110

Towards chains of tunable and nonlinear superconducting microwave resonators — •Michael Fischer[1,2], Friedrich Wulschner[1,2], Udo Schaumburger[1,2], Max Haeberlein[1,2], Manuel Schwarz[1,2,3], Peter Eder[1,2,3], Edwin Menzel[1,2,3], Kirill Fedorov[1,2], Jan Goetz[1,2], Edwar Xie[1,2], Ling Zhong[1,2,3], Frank Deppe[1,2,3], Achim Marx[1], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

We present an experimental feasibility study of chains of tunable and nonlinear superconducting microwave resonators within the realm of circuit QED. We describe the fabrication and experimental characterization of the components required to realize nonlinear resonators with tunable anharmonicity, capacitively coupled resonator chains and on-chip parallel plate capacitors. We discuss possible error sources in the fabrication and characterization processes. Furthermore, simulations based on existing theories are performed to identify accessible parameter ranges.

This work is supported by the DFG via SFB 631 and the EU projects CCQED and PROMISCE.

TT 16.8 Mon 16:45 H 0110

Probing the Interaction of Microscopic Material Defects with Quasiparticles using a Superconducting Qubit — •Alexander Bilmes[1], Jürgen Lisenfeld[1], Andreas Heimes[2], Sebastian Zanker[2], Gerd Schön[2], Georg Weiss[1], and Alexey V. Ustinov[1] — [1]PI, Fakultät für Physik, KIT, Wolfgang-Gaede-Straße 1, 76131 Karlsruhe, Germany — [2]TFP, Fakultät für Physik, KIT, Wolfgang-Gaede-Straße 1, 76131 Karlsruhe, Germany

Two-Level-Systems (TLS) are one of the main sources of decoherence in superconducting nano-scale devices such as SQUIDs, photon detectors, resonators and quantum bits (qubits), although the TLS' microscopic nature remains unclear. We use a superconducting phase qubit to detect TLS contained within the tunnel barrier of the qubit's Josephson junction. We coherently operate *individual* TLS by resonant microwave pulses and access their quantum state by utilizing their strong coupling to the qubit. Our previous measurements of TLS coherence in dependence of the temperature indicate that quasiparticles may give rise to TLS energy loss and dephasing. Here, we probe the TLS-quasiparticle interaction using a reliable method of *in-situ* quasiparticle injection via an on-chip dc-SQUID that is pulse-biased beyond its critical current. The quasiparticle density is calibrated by measuring associated characteristic changes to the qubit's resonance frequency and energy relaxation rate [1]. We will present experimental data that clearly show the influence of quasiparticles on TLS coherence.

[1] M. Lenander et al., Phys.Rev. B 84, 024501 (2011).

TT 16.9 Mon 17:00 H 0110

Incoherent Two-Level Fluctuators inside the Josephson junction of a Superconducting Qubit — •Saskia Meissner, Jürgen Lisenfeld, Alexey V. Ustinov, and Georg Weiss — Physikalisches Institut, KIT Karlsruhe

Spectroscopy on qubits based on Josephson junctions reveals the precence of defects like quantum coherent tunneling systems (TS) as well as two-level fluctuators (TLF). TLF are incoherent tunneling particles which are described by dissipative quantum tunneling theory. Due to the coherent interaction of qubit and the TS, it is possible to probe individual TLF that themselves are coupled to a tunneling system.

Here we perform high resolution defect spectroscopy by tuning the TS and TLF asymmetry energies with external strain applied to the qubit chip. Slow fluctuators induce telegraph noise in the resonance frequency of TS. Fast fluctuators create double resonances of TS in the manner of two frequency branches. Apparently, the two-level fluctuator causes a rapid modulation of the asymmetry energy of the tunneling system on top of the static strain tuning. We perform time domain analyses of TS resonance frequencies with the goal of reconstructing the TLF deformation potential and the TLF-TS interaction potentials.

TT 17: Superconductivity: Properties and Electronic Structure

Time: Monday 15:00–18:45 Location: H 2053

TT 17.1 Mon 15:00 H 2053

Broadband microwave response of superconducting NbN and TaN thin films — M. Maximilian Felger[1], Uwe S. Pracht[1], Martin Dressel[1], Konstantin Ilin[2], Michael Siegel[2], and •Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, D-70669 Stuttgart, Germany — [2]Institut für Mikro- und Nanoelektronische Systeme, Karlsruher Institut für Technologie, D-76187 Karlsruhe, Germany

Ultrathin NbN and TaN films with their peculiar superconducting behavior are of interest both for fundamental physics (e.g. concerning the superconductor-insulator transition) and novel applications (e.g. for single-photon detectors). Here microwave spectroscopy is a powerful tool to characterize essential superconducting properties and to investigate the charge dynamics (Cooper pairs and quasiparticles).

We have prepared by sputtering thin films of NbN (thickness between 3 nm and 20 nm; T_c between 5 K and 13 K) and TaN (thickness 5 nm; T_c between 8.5 K and 9.5 K) on sapphire substrates. We performed broadband microwave spectroscopy on these samples using a Corbino spectrometer at temperatures down to 1.1 K and at frequencies up to 50 GHz. From these data we determine the superconducting penetration depth and we evaluate the frequency-dependent conductivity. While many of the observed features can be described within expectations of conventional BCS theory, we also find deviations that are caused by fluctuations near the superconducting transition.

TT 17.2 Mon 15:15 H 2053

Magnetic field dependence of the superconducting proximity effect in a two atomic layer thin metallic film — Michael Caminale, Augusto A. Leon Vanegas, Agniezka Stepniak, Hirofumi Oka, •Jeison A. Fischer, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle

The intriguing possibility to induce superconductivity in a metal, in direct contact with a superconductor, is under renewed interest for applications and for fundamental aspects [1]. The underlying phenomenon is commonly known as proximity effect. In this work we exploit the high spatial resolution of scanning tunneling spectroscopy at sub-K temperatures and in magnetic fields. We probe the differential conductance along a line from a superconducting 9 ML high Pb nanoisland into the surrounding two layer thin Pb/Ag wetting layer on a Si(111) substrate. A gap in the differential conductance indicates superconductivity of the Pb island. We observe an induced gap in the wetting layer, which decays with increasing distance from the Pb island. This proximity length is 21 nm at 0.38 K and 0 T. We find

a non-trivial dependence of the proximity length on magnetic field. Surprisingly, we find that the magnetic field does not affect the induced superconductivity up to 0.3 T. However, larger fields of 0.6 T suppress superconductivity in the wetting layer, where the Pb island still remains superconducting. We discuss the unexpected robustness of induced superconductivity in view of the high electronic diffusivity in the metallic wetting layer.

[1] Guéron et al. Phys. Rev. Lett. 77, 3025 (1996);
Xiang et al. Nat. Nano. 1, 208 (2006);
Wang et al. Phys. Rev. Lett. 100, 197002 (2008).

TT 17.3 Mon 15:30 H 2053

Scanning tunneling spectroscopy of Co adsorbates on superconducting Pb nanostructures — •Regis Decker, Michael Caminale, Hirofumi Oka, Agneszka Stepniak, Augusto A. Leon Vanegas, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

Superconductivity in low-dimensional structures has become an active research area [1,2]. In order to understand the superconducting pairing, long-standing work has been devoted to the pair breaking effect, where magnetic impurities break Cooper pair singlets [3]. We performed scanning tunneling spectroscopy at low temperature on Co adsorbates on superconducting Pb nanoislands. On the Co adsorbates, we observe spectral features in the superconductor's energy gap, which we attribute to magnetic impurity induced bound states [3], a hallmark of the pair breaking effect. We discuss the response of the superconducting islands to the presence of Co adsorbates.

[1] T. Nishio et al., Phys. Rev. Lett. 101, 167001 (2008).
[2] T. Zhang et al., Nature Phys. 6, 104 (2010).
[3] A. V. Balatsky et al., Rev. Mod. Phys. 78, 373 (2006).

TT 17.4 Mon 15:45 H 2053

Suppression of superconductivity in a single Pb layer on Ag/Si(111) — •Augusto Leon-Vanegas[1,2], Michael Caminale[1], Agnieszka Stepniak[1], Hirofumi Oka[1], Antonio Sanna[1], Andreas Linscheid[1], Dirk Sander[1], and Jürgen Kirschner[1,2] — [1]Max Plank Institüt für Mikrostukturphysik — [2]Martin Luther Univeristät, Halle-Wittenberg

Recently, superconductivity was reported in a single layer of Pb on Si(111) with a critical temperature of 1.83 K [1]. It has been proposed that the interaction of Pb with the Si substrate provides the electron phonon coupling to support superconductivity in this system [2]. We have used a ^{3}He-cooled STM with a vector magnetic field to study the effect of insertion of a Ag interlayer on the superconducting properties of a single Pb layer on Si(111). In contrast to the experiments on Pb/Si(111), the differential conductance of Pb/Ag/Si(111) does not show a gap indicative of superconductivity even at the lowest experimental temperature of 0.38 K. We ascribe this to the suppression of superconductivity [3]. This result is explained by means of ab-initio calculations, showing that the effect of a chemical hybridization between Pb and Ag/Si occurring at the Fermi level dramatically reduces the strength of the electron phonon coupling. This contrasts with the case of Pb/Si(111), where no overlap between Pb and Si electronic states at the Fermi level is found in the calculations.

[1] Zhang et al., Nat. Phys. 6, 104 (2010)
[2] Noffsinger and Cohen, Sol. State Comm. 151, 421 (2011)
[3] Stepniak, et al., J. Surface and Interface Analysis(2014)

TT 17.5 Mon 16:00 H 2053

Signatures of Unconventional Superconductivity in Granular Aluminum — •Uwe S. Pracht[1], Nimrod Bachar[2,3], Eli Farber[2], Guy Deutscher[3], Martin Dressel[1], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Laboratory for Superconductivity and Optical Spectroscopy, Ariel University, Israel — [3]Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Israel

Thin films composed of nanoscale Al grains coupled through dielectric barriers exhibit peculiar superconducting properties: As the grain coupling is decreased, the normal-state resistivity ρ increases and the critical temperature T_c is elevated from 1.1 K to 3.2 K before it is suppressed to zero at a critical ρ_c. This dome-like appearence of superconductivity together with Kondo-like normal-state transport and presence of localized spins suggest the superconducting mechanism to be of unconventional type in contrast to the BCS nature of bulk Al.

We measured the dynamical conductivity $\hat{\sigma}(\nu) = \sigma_1(\nu) + i\sigma_2(\nu)$ in the range 90 - 700 GHz of various films with different ρ by means of quasi-optical Mach-Zehnder interferometry above and below T_c. With increasing ρ we find an enhanced sub-gap absorption compared to the BCS theory for $\sigma_1(\nu)$ which we discuss in various contexts such as collective modes or magnetic impurity scattering, [1,2].

[1] N. Bachar, U. S. Pracht *et al.*, J. Low Temp. Phys (in print)
[2] D. Sherman, U. S. Pracht *et al.*, Nat. Phys (accepted)

TT 17.6 Mon 16:15 H 2053

Long-ranged interactions in thin TiN films at the superconductor-insulator transition? — •Klaus Kronfeldner[1], Tatyana Baturina[2], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]A. V. Rzhanov Institute of Semiconductor Physics SB RAS, Novosibirsk 630090, Russia

We measured IV-characteristics and magnetoresistance of square TiN-films in the vicinity of the disorder-tuned superconductor-insulator transition (SIT) for different sizes (5μm to 240μm). While the films are superconducting at zero magnetic field, at finite fields a SIT occurs. The resistance shows thermally activated behaviour on both sides of the SIT. Deep in the superconducting regime the activation energy grows linear with the sample size as expected for a size-independent critical current density. Closer to the SIT the activation energy becomes clearly size independent. On the insulating side the magnetoresistance maximum and the activation energy both grow logarithmically with sample size which is consistent with a size-limited charge BKT (Berezinskii-Kosterlitz-Thouless) scenario. In order to test for the presence of long-ranged interactions in our films, we investigate the influence of a topgate. It is expected to screen the possible long-ranged interactions as the distance of the film to the gate is much shorter than the electrostatic screening length deduced from the size-dependent activation energy.

TT 17.7 Mon 16:30 H 2053

Multigap superconductivity with broken time reversal symmetry in locally noncentrosymmetric SrPtAs — •Felix Brückner[1], Hubertus Luetkens[2], Hannes Kühne[3], Pabitra Kumar Biswas[2], Titus Neupert[4], Marco Günther[1], Rajib Sarkar[1], Tobias Stürzer[5], Dirk Johrendt[5], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, Technische Universität Dresden, Germany — [2]Paul-Scherrer-Institut, Villigen, Switzerland — [3]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [4]Princeton Center for Theoretical Science, Princeton University, Princeton, USA — [5]Ludwig-Maximilians-Universität München, Germany

The recently discovered compound SrPtAs has awakened grown scientific interest, because it comprises an exceptional structural feature: it consists of non-centrosymmetric PtAs layers that are weakly coupled to each other. Thus, SrPtAs is a prime example for staggered noncentrosymmetricity. Theoretical calculations predict an unconventional chiral *d*-wave superconducting state which is unique in material science, but no general consent has been archieved.

The evidence for time reversal symmetry breaking was found in μSR experiments, which implies an unconventional superconducting state. Nuclear quadrupole resonance reveals multigap behavior and a fully gapped superconducting state. In particular, I present spin-lattice relaxation rate ($1/T_1$) measurements and discuss possible pairing symmetries. These results are relevant to understand the pairing mechanism in this and similar compounds. While the fokus is on the experiment, I will discuss the theoretical point of view as well.

TT 17.8 Mon 16:45 H 2053

Light induced superconductivity in underdoped $YBa_2Cu_3O_x$ — •Stefan Kaiser[1,2,3], Daniele Nicoletti[1], Cassi Hunt[1], Wanzheng Hu[1], Roman Mankowsky[1], Michael Först[1], Isabella Gierz[1], Toshinao Loew[2], Mathieu LeTacon[2], Bernhard Keimer[2], and Andrea Cavalleri[1] — [1]Max-Planck-Institut für die Struktur und Dynamik der Materie, Hamburg — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart — [3]4. Physikalisches Institut und Research Center SCoPE, Uni Stuttgart

Photo-stimulation with femtosecond mid-infrared pulses allows us to induce an inhomogeneous non-equilibrium superconducting state in $YBa_2Cu_3O_x$ at temperatures as high as 300 K. Its transient response is probed via THz time-domain spectroscopy [1,2]. We measure and characterize its complex optical response above and below the superconducting transition temperature T_c: Below T_c, we find an enhancement of the optical signatures of superconducting coherence. Above T_c we find that the incoherent optical properties at equilibrium be-

come highly coherent with optical signatures very similar to the ones for superconductors below T_c. In the course of understanding these observations, ultrafast x-ray experiments at LCLS allow us observing reconstructed crystal structure in the transient superconducting state and the influence of competing CDW-order to the phonon-excitation [3,4].

[1] S. Kaiser et al., PRB 89, 184516 (2014).
[2] W. Hu et al., Nat. Mat. 13, 705 (2014).
[3] R. Mankowsky et al., arXiv:1405.2266.
[4] M. Först et al., PRB 90, 184514 (2014).

15 min. break.

TT 17.9 Mon 17:15 H 2053

The evolution of microwave conductivity in $YBa_2Cu_3O_{6+x}$ across the superconducting dome — •Jordan Baglo[1], James Day[2], Pinder Dosanjh[2], Ruixing Liang[2], Walter Hardy[2], and Doug Bonn[2] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom — [2]Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada

The rich phenomenology displayed in the phase diagram of the high-T_c cuprates continues to be an active arena of investigation. Recent experimental and theoretical work appears to be converging on a picture of separate spin and charge order phase transitions – well-below and near optimal doping, respectively – along with associated Fermi surface reconstruction. As sensitive probes of the low-energy electrodynamics, microwave spectroscopy techniques are well-suited for characterizing the effects of such changes in electronic structure deep within the superconducting state.

I will present the results of our survey of the complex microwave conductivity of $YBa_2Cu_3O_{6+x}$ over a wide range of oxygen contents, from 6.49 to 6.998, and discuss their implications for the evolution of electronic structure with doping. In particular, I will highlight the apparent absence of a peak in penetration depth near the proposed $p \approx 0.18$ quantum critical point (QCP), contrasting with its presence near the antiferromagnetic QCP of the pnictide superconductors. I will also discuss the surprising relationship we observed between quasiparticle scattering lifetimes and oxygen ordering, which carries important implications for quantum oscillation measurements.

TT 17.10 Mon 17:30 H 2053

Charge density wave fluctuations in $La_{2-x}Sr_xCuO_4$ and their competition with superconductivity — •Thomas Croft[1], Christopher Lester[1], Alessandro Bombardi[2], Mark Senn[2], and Stephen Hayden[1] — [1]H. H. Wills Physics Laboratory, University of Bristol, Bristol, BS8 1TL, United Kingdom — [2]Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, United Kingdom

The recent observations of charge and stripe correlations in $YBa_2Cu_3O_{6+x}$ and $La_{2-x}Ba_xCuO_4$ has reinvigorated interest in their role in influencing the superconductivity of the cuprates. However, structural complications of these systems makes it difficult to isolate the effect the lattice has in inducing the charge order.

Here, we report hard x-ray diffraction measurements on three compositions ($x = 0.11, 0.12, 0.13$) of the high-temperature superconductor $La_{2-x}Sr_xCuO_4$, a canonical example of HTS with $T_c \approx 35$ K and a simple crystal structure. All samples show charge-density-wave (CDW) order with onset temperatures in the range 51-80 K and ordering wavevectors close to (0.23,0,0.5). We present a phase diagram of $La_{2-x}Sr_xCuO_4$ including the pseudogap phase, CDW and magnetic order.

TT 17.11 Mon 17:45 H 2053

Microstructural characterization of Bulk MgB_2 — •Alex Wiederhold[1], Michael Koblischka[1], Kazuo Inoue[2], Miryala Muralidhar[2], Masato Murakami[2], Kévin Berger[3], Bruno Douine[3], Thomas Hauet[4], Jacques Noudem[5], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, Saarland University, P. O. Box 151150, D-66123 Saarbrücken, Germany — [2]Department of Material Science and Engeneering, Shibaura Institute of Technology, 3-7-5 Toyosu, Koto-ku, Tokyo 135-8548, Japan — [3]GREEN, Université de Lorraine, Vandœuvre-les-Nancy, France — [4]Institute Jean Lamour, Université de Lorraine, Vandœuvre-les-Nancy, France — [5]CRISMAT-CNRS, Cherbourg, France

A series of disk-shaped bulk MgB_2 superconductors (sample diameter up to 4 cm) was prepared in order to improve the performance for superconducting super-magnets. Several samples were fabricated using a solid state reaction in pure Ar atmosphere from 750 to 950 °C to obtain the highest critical current density (j_c) as well as large trapped field values. Magnetization and transport measurements revealed that at the low reaction temperatures flux pinning at grain boundaries is dominant, which is decreasing on increasing temperature. At the highest reaction temperature, j_c was found to increase again indicating a change of the pinning mechanism [1]. In order to clarify this behavior the samples were characterized in detail by means of transmission electron microscopy (TEM) and transmission electron backscatter diffraction (t-EBSD).

[1] M.R.Koblischka *et al.*, IEEE Trans. Magn. (in press).

TT 17.12 Mon 18:00 H 2053

Magnetic characterization of Ag-addet Bulk MgB_2 — •Alex Wiederhold[1], Michael Koblischka[1], Kazuo Inoue[2], Miryala Muralidhar[2], Masato Murakami[2], Thomas Hauet[3], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, Saarland University, P. O. Box 151150, D-66123 Saarbrücken, Germany — [2]Department of Material Science and Engeneering, Shibaura Institute of Technology, 3-7-5 Toyosu, Koto-ku, Tokyo 135-8548, Japan — [3]Institute Jean Lamour, Université de Lorraine, Vandœuvre-les-Nancy, France

n earlier studies, it was found that bulk sintered MgB_2 samples contained numerous voids which hinder the current flow. Therefore, a series of bulk MgB_2 superconductors with Ag contents of 0-10 wt% was prepared in order to improve the critical current densities and the mechanical performance. Several samples were fabricated using a solid state reaction in pure Ar atmosphere at the optimal reaction temperature of 775 °C. Thorough microstructural observations obtained from scanning electron microscopy (SEM) and atomic force microscopy (AFM) indicate that metallic Ag particles are embedded in the void regions.Furthermore, nanometer-sized $AgMg_3$ particles are also present within the MgB_2 matrix, leading to improved flux pinning. Small samples cut from the bulks were characterized by transport measurements ($R(T, B)$ and I/V characteristics) in magnetic fields up to 8 T and by magnetization loops measured using a SQUID magnetometer.

TT 17.13 Mon 18:15 H 2053

Umkehr effect observed in the magnetothermoelectric power of graphite — •Santiago Muiños-Landin, Israel Lorite Villalba, Winfried Böhlmann, and Pablo Esquinazi — Division of Superconductivity and Magnetism, Institute for experimental Physics II, Fakultät für Physik und Geowissenschaften, Linnéstrasse 5, 04103 Leipzig, Germany

In thermoelectricity, the Umkehr effect is defined as the difference between the the Seebeck coeffcient values upon reversal of an applied magnetic field. It was shown to be very large for certain samples of the semimetal bismuth. We show here that the effect is also observed in highly oriented pyrolytic graphite(HOPG Union Carbide), while it is not for a HOPG sample of a different provider. The only difference between these two samples is the amount of well deffined two-dimensional interfaces that exist inside them. The contribution to the thermoelectric power (TEP) that comes only from the graphite interfaces, makes non symmetric the response of the Seebeck effect once the sign of the magnetic field is changed. This fact provides an explanation for the Umkehr effect in graphite, in terms of the contribution of the interfaces to the TEP in our samples. Recently published work indicates that granular superconductivity is embedded in some of the interfaces. Therefore, we may now speculate that the extra entropy contribution to the magnetothermoelectric effect may be due to some kind of vortices produced by the applied magnetic field at the superconducting regions. We correlate therefore the field dependence of this contribution and its temperature dependence with that of the magnetoresistance.

TT 17.14 Mon 18:30 H 2053

Elucidating superconductivity and intermediate valence of elemental Eu under high pressure — •Jürgen Röhler — Universität zu Köln, 50937 Köln, Germany

Elemental Eu is a superconductor under high pressure, $P \geq 80$ GPa, up to $T_c = 2.75$ K at 142 GPa [1]. We elucidate the possible connection between pressure induced $4f$ configurational changes, $Eu^{2+}(4f^7, J{=}7/2) \rightleftarrows Eu^{3+}$ $(4f^6, J{=}0)$, and superconductivity. Notably high pressure L_{III} XAS [2] and more recently also ME isomer shift measurements [3] do not show the theoretically expected 2^+ - 3^+ transition, but interme-

diate valence states saturating at $v \simeq 2.6$ between ~ 20 and 70 GPa, and undergoing between 31 and 37 GPa a transformation into a complex incommensurately modulated monoclinic structure $\sim \alpha$-U, which is followed by an other hitherto unidentified low-symmetry complex structure. We discuss how the Brillouin zone - Fermi surface interaction, driven by the non integer valence electron count, may stabilize low-symmetry complex structures, which tend to favor the occurrence of superconductivity through bandstructures with overlapping electron and hole bands.

[1] M. Debessai *et al.*, Phys. Rev. Lett. **102**, 197002 (2009).
[2] J. Röhler, Physica **144B**, 27 (1986).
[3] W. Bi *et al.*, Phys. Rev. B **85**, 205134 (2012).

TT 18: Correlated Electrons: Spin Systems and Itinerant Magnets – Frustrated Magnets 2 (jointly with MA)

Time: Monday 15:00–18:30 Location: H 3005

TT 18.1 Mon 15:00 H 3005

Semionic resonating valence bond states — •Mohsin Iqbal[1], Didier Poilblanc[2], and Norbert Schuch[1] — [1]JARA Institute for Quantum Information, RWTH Aachen, 52056 Aachen, Germany — [2]Laboratoire de Physique Theorique, C.N.R.S. and Universite de Toulouse, 31062 Toulouse, France

Ground state of Heisenberg antiferromagnet (HAFM) on kagome lattice forms a Z2 topological spin liquid. However, the topological nature of the spin liquid is not entirely clear. We propose semionic resonating valence bond (RVB) states as an ansatz to characterize the topological order using the formalism of Projected Entangled Pair States (PEPS). In contrast to normal resonating valence bond state (proposed in earlier studies as another ansatz) which is in the phase of Kiteav toric code, semionic RVB states carry the topological order of double semion model.

Within PEPS formalism one can extend the ansatz and construct semionic simplex RVB states. Variational calculations show that semionic simplex RVB states give relatively lower energy for HAFM on kagome lattice compared to simplex RVB states and make a better candidate to describe the topological order.

TT 18.2 Mon 15:15 H 3005

Exotic magnetization plateaus in a quasi-two-dimensional Shastry-Sutherland model — Gregor Foltin[1], •Salvatore R. Manmana[2], and Kai P. Schmidt[1] — [1]Lehrstuhl f. Theoretische Physik 1, TU Dortmund, D-44221 Dortmund — [2]Institut f. Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen

We find unconventional Mott insulators in a quasi-2D version of the Shastry-Sutherland model in a magnetic field. In our realization on a four-leg tube geometry, these are stabilized by correlated hopping of localized magnetic excitations. Using perturbative continuous unitary transformations (pCUTs, plus classical approximation or exact diagonalization) and the density matrix renormalisation group method (DMRG), we identify prominent magnetization plateaus at magnetizations $M = 1/8$, $3/16$, $1/4$, and $1/2$. While the plateau at $M = 1/4$ can be understood in a semiclassical fashion in terms of diagonal stripes, the plateau at $M = 1/8$ displays highly entangled wheels in the transverse direction of the tube. Finally, the $M = 3/16$ plateau is most likely to be viewed as a classical $1/8$ structure on which additional triplets are fully delocalized around the tube. The classical approximation of the effective model fails to describe all these plateau structures which benefit from correlated hopping. We relate our findings to the full 2D system, which is the underlying model for the frustrated quantum magnet $SrCu(BO_3)_2$.

TT 18.3 Mon 15:30 H 3005

Weyl spin liquids — •Kevin O'Brien, Maria Hermanns, and Simon Trebst — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

Topological semimetals – the gapless cousins of topological insulators – have attracted much recent interest. They exhibit bulk features such as gapless Weyl nodes that can be characterized by topological invariants. In addition, they possess gapless surface modes, also called Fermi arcs, which are intimately connected to the bulk features and, thus, topologically protected.

Here we discuss the emergence of such a topological semimetal in three-dimensional generalizations of the Kitaev model. These models describe the fractionalization of spin-orbit entangled moments into Majorana fermions and a $\mathbb{Z}_2$ gauge field. We demonstrate that the Majorana fermions form a Weyl superconductor for the Kitaev model on the recently synthesized hyperhoneycomb structure of β-Li_2IrO_3 in the presence of an external magnetic field. We discuss the topologically protected bulk and surface features of this state, which we dub a Weyl spin liquid.

TT 18.4 Mon 15:45 H 3005

Orphan glassiness in a disordered spin liquid — •Jorge Armando Rehn[1], Arnab Sen[2], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Indian Association for the Cultivation of Science, Kolkata

The random dilution of non-magnetic impurities in systems presenting a classical spin liquid phase leads to interesting new physics: certain spins in direct proximity to vacancies are known to be fractionalized, and to create an extended spin texture on its neighborhood. A mapping of the pure spin system to a distribution of fluxes living on a dual bipartite lattice enables understanding of the thermal excitations as emerging Coulomb charges. Using this mapping it is also possible to interpret the diluted system in terms of charges, which are not entropically generated, but induced by the vacancies. The effective picture obtained at low temperatures for the diluted system neglects entropically generated charges and considers only the randomly placed long ranged interacting charges induced by the vacancies. A study of this effective model and the possibility of a glassy phase in this system will be presented on this talk.

TT 18.5 Mon 16:00 H 3005

Majorana metals and quantum spin liquids — •Maria Hermanns, Kevin O'Brien, and Simon Trebst — Institute for Theoretical Physics, Cologne, Germany

One of the most intriguing phenomena in strongly correlated systems is the fractionalization of quantum numbers – familiar examples include the spin-charge separation in one-dimensional metallic systems, the fractionalization of the electron in fractional quantum Hall states or the emergence of monopoles in spin ice.

In this talk, I will discuss the fractionalization of magnetic moments in spin-orbit entangled j=1/2 Mott insulators, in which the emergent degrees of freedom are Majorana fermions. The latter form metallic states whose precise character intimately depends on the underlying lattice structure. The origin of such dichotomous states is elucidated by a family of exactly solvable Kitaev-type models of frustrated quantum magnets in three dimensions, which might be realized in a class of recently synthesized Iridate compounds. In particular, these models provide the first analytical tractable examples of long sought-after quantum spin liquids with a spinon Fermi surface and even an entire new class of quantum spin liquids – so-called Weyl spin liquids, in which the fractionalized degrees of freedom form a topological Weyl-superconductor.

TT 18.6 Mon 16:15 H 3005

Magnetic monopoles in diluted quantum spin ice — •Olga Petrova[1], Roderich Moessner[1], and Shivaji Sondhi[2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Princeton University, Princeton, NJ, USA

Typical spin ice materials can be modeled using classical Ising spins. The geometric frustration of the pyrochlore lattice causes the spins to satisfy ice rules, whereas a violation of the ice constraint constitutes an excitation. Flipping adjacent spins fractionalizes the excitation into two monopoles. Long range dipolar spin couplings result in Coulombic interactions between charges, while the leading effect of quantum fluctuations is to provide the monopoles with kinetic energy. We study weakly diluted spin ice including the leading effects of quantum mechanical fluctuations. We find that a missing spin gives rise to hydrogenic excited states in which a magnetic monopole is bound to the vacancy at various radii. We compute the properties of these states

via a mapping to a single particle problem that is defined on the Bethe lattice. These quantities are then used to obtain an expression for the dynamic structure factor, that can be measured in neutron scattering experiments directly.

TT 18.7 Mon 16:30 H 3005

Monte-Carlo Study of Polarization Plateaux in Hexagonal Water Ice — •Matthias Gohlke, Frank Pollmann, and Roderich Moessner — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We study the hexagonal phase Ih of water ice in an external electric field at low temperatures using a Worm Monte Carlo algorithm. We observe polarization plateaux when the field is aligned along the [001] and [1-10] directions. In each case, one plateau occurs at intermediate polarization with finite entropy. The remaining degrees of freedom can be mapped to dimer models on the honeycomb and the square lattice, respectively. Upon slightly tilting the external field, we observe a Kasteleyn transition to a plateau with saturated polarization and vanishing entropy. This transition is checked analytically using the Pfaffian method and compared to the Monte Carlo results.

15 min. break.

TT 18.8 Mon 17:00 H 3005

Comparison between dynamical permeability and permittivity in $Dy_2Ti_2O_7$ at low temperatures — •Steffen Harms[1], Christoph P. Grams[1], Martin Valldor[2], and Joachim Hemberger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

$Dy_2Ti_2O_7$ if one of the well known spin-ice compounds in which magnetic monopoles are emergent [1]. It was predicted, that these monopoles carry electric dipole moments [2] and therefore the monopole dynamics can be seen in the dielectrical response $\varepsilon^*(\nu)$.
Recently published data exhibits the speeding up of a dielectric relaxation process reaching a relaxation rate of up to $\nu_0 = 100$ kHz near the critical-endpoint of the (H,T)-phase diagram [3]. This process can be associated with the hopping of magnetic monopoles and should among other contributions also be seen in the magnetic ac-susceptibility.
Here we present a comparative broadband study of complex permittivity and permeability in the mK range in order to disentangle the different contributions to the dynamic response in the spin-ice $Dy_2Ti_2O_7$.

Funded through the Institutional Strategy of the University of Cologne within the German Excellence Initiative and research grant HE-3219/2-1.

[1] C. Castelnovo et al., Nature 451, 42 (2008).
[2] D. I. Khomskii, Nature Communications 3, 1 (2012).
[3] C. P. Grams et al., Nature Communications 5, 4853 (2014).

TT 18.9 Mon 17:15 H 3005

Groundstate Entropy and Monopole Heat Transport in dilute Spin Ice — •S. Scharffe[1], G. Kolland[1], M. Valldor[1,2], O. Breunig[1], J. F. Welter[1], P. Laschitzky[1], and T. Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

The spin ice $Dy_2Ti_2O_7$ is a geometrically frustrated spin system consisting of corner-sharing tetrahedra. An Ising anisotropy aligns the spins along their local easy axes in the {111} directions. Possible groundstates are given by the "ice-rule": two spins point into and two out of each tetrahedron. This behavior is analogous to the hydrogen displacement in water ice, revealing a residual entropy for $T \to 0$ K. Anomalous excitations are created by single spin flips and are discussed as magnetic monopoles which contribute to the magnetic heat transport in spin ice[1, 2]. Here, specific heat and heat transport measurements of the pure spin ice and the diluted reference materials $(Dy_{1-x}Y_x)_2Ti_2O_7$ are presented. We extract c_{mag} and demonstrate how the residual entropy of the pure spin ice varies with increasing non-magnetic Y-dilution. Additionally, we show that the monopole contribution κ_{mag} to the total heat transport also correlates with the degree of Y-dilution. The extraction of κ_{mag} and c_{mag} enables us to calculate the magnetic diffusion coefficient D_{mag} of the spin-ice materials which is strongly suppressed in the diluted systems for $T < 1$ K.

This work was supported by the DFG via project LO 818/2-1.

[1] Kolland *et. al.*, Phys. Rev. B, **86**, 060402(R) (2012)
[2] Scharffe *et. al.*, J. Magn. Magn. Mater. (in press, arXiv:1406.4037).

TT 18.10 Mon 17:30 H 3005

Non-linear susceptibility of spin ice from the Wien effect — •Vojtěch Kaiser[1,2], Steven T. Bramwell[3], Peter C.W. Holdsworth[2], and Roderich Moessner[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]École normale supérieure de Lyon, Lyon, France — [3]London Centre for Nanotechnology, University College London, London, UK

We give predictions for the non-linear magnetic response of the emergent Coulomb fluid of magnetic monopoles in spin ice. To this end, we combine the increase of the monopole density due to the second Wien effect with the magnetization dynamics of spin ice. Non-linearities that occur thanks to this coupling between monopoles and spins manifest themselves in computer simulations and are explained by a simple kinetic model. At longer times, spin ice magnetizes which renders the density increase transient unless the field direction is changed periodically. Strikingly, for certain frequencies the non-equilibrium non-linear response due to the Wien effect in spin ice is indistinguishable from an electrolyte. Studying the response to harmonic driving with large amplitude allows us to define a non-linear susceptibility of spin ice as a potential experimental signature of these phenomena.

TT 18.11 Mon 17:45 H 3005

Field Induced Phases and Possible Multimagnon Bound States in the Frustrated Quantum Spin Chain Linarite — Britta Willenberg[1], Manfred Reehuis[1], Markus Schäpers[2], Anja U.B. Wolter[2], Stefan.-Ludwig Drechsler[2], Satoshi Nishimoto[2], Bernd Büchner[2], Kirrily C. Rule[3], Bachir Ouladdiaf[3], and •Stefan Süllow[4] — [1]HZ Berlin, Berlin, Germany — [2]IFW Dresden, Dresden, Germany — [3]The Bragg Institute, ANSTO, Australia — [4]IPKM, TU Braunschweig, Braunschweig, Germany

A neutron diffraction and NMR study of the field induced phases of linarite $PbCuSO_4(OH)_2$ is presented for magnetic fields $H \parallel b$ axis at temperatures down to 1.7 K. A two step spin flop transition is observed, transforming the helical magnetic ground state into a collinear structure. As well, a magnetic phase with sine-wave modulated moments parallel to the field direction was detected, enclosing the other long-range ordered phases. The propagation vector of this 3D spin density wave phase shifts with increasing magnetic field. Theoretical calculations imply that linarite possesses an xyz exchange anisotropy. Within this model a coexistence of 2-, 3-, and 4- magnon bound states is predicted to be present in linarite.

TT 18.12 Mon 18:00 H 3005

High-temperature heat transport in coupled quantum spin chains — •Christian Hess[1], Oleg Mityashkin[1], Ashwin Mohan[1], Chinnathambi Sekar[1], Gernot Krabbes[1], Bernd Büchner[1], Romuald Saint-Martin[2], and Alexandre Revcolevschi[2] — [1]Institute for Solid State Research, IFW Dresden, 01069 Dresden, Germany — [2]Laboratoire de Physico-Chimie de L'Etat Solide, Université Paris-Sud, 91405 Orsay, France

We present high-temperature heat conductivity data up to $T \sim J/2k_B$ for the compounds $SrCuO_2$ and $CaCu_2O_3$, which represent spin-1/2 realizations of the isotropic Heisenberg spin chain and of a weak-rung two-leg spin ladder, respectively. In both cases, the high-temperature heat conductivity is suppressed with increasing temperature, which indicates a thermally activated scattering process. Indeed, the analysis of the data reveals a perfect description of the temperature dependence of the mean free path l_{mag} by just two scattering processes, viz. (i) a temperature independent scattering off boundaries that dominates at low temperature, and (ii) thermally activated high-temperature scattering $l_{\mathrm{mag}} \sim \exp(-T^*/T)$. Interestingly, for the Heisenberg spin chain the energy scale k_BT^* of the activated scattering is comparable with typical phonon energies, suggestive of spinon-phonon scattering. However, in the weak-rung spin ladder, which can be viewed as a pair of weakly coupled spin chains, the energy scale of the activated scattering is clearly beyond the phonon energies in the system and $k_BT^* \sim J$. These findings suggest that the weak interchain coupling introduces a new, magnetic type of scattering.

TT 18.13 Mon 18:15 H 3005

Spin structures of S = 5/2 antiferromagnetic triangular lattices: $AAg_2M[VO_4]_2$ — •Angela Möller[1], Clarina R. de la Cruz[2], Ngozi E. Amuneke[1], and Joshua Tapp[1] — [1]Department of Chemistry and TcSUH, University of Houston, United States — [2]Quantum Condensed Matter Division, ORNL, Oak Ridge, United States

The $AAg_2M[VO_4]_2$ compounds present a unique series for studying structure-property relationships. The size of the A cation (Ba^{2+}, K^+, Rb^+, or Ag^+) controls i) the inter-layer distances between the magnetic triangular lattices (M, here Mn^{2+} or Fe^{3+}) and ii) the distortion of the non-magnetic vanadate units. The crystal and magnetic structures were refined from neutron diffraction data under applied fields (ORNL, HB2A) and reveal the complex magnetic phase diagrams of frustrated S=5/2 triangular lattices with axial and XY-anisotropy, respectively [1].

This work was supported by the National Science Foundation (DMR-1149899) and by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy.

[1] N. E. Amuneke, et al., Chem. Mater. 26, 5930 (2014).

TT 19: Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 2 (jointly with DY)

Time: Monday 15:00–18:00 Location: H 3010

TT 19.1 Mon 15:00 H 3010

Quenching the Anisotropic Heisenberg Chain: Exact Solution and Generalized Gibbs Ensemble Predictions — •Bram Wouters[1], Jacopo De Nardis[1], Michael Brockmann[1], Davide Fioretto[1,2], Marcos Rigol[3], Rogier Vlijm[1], and Jean-Sébastien Caux[1] — [1]Institute for Theoretical Physics, University of Amsterdam, Science Park 904, Postbus 94485, 1090 GL Amsterdam, Netherlands — [2]Institute for Theoretical Physics, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [3]Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA

We study quantum quenches in integrable spin $\frac{1}{2}$ chains in which we evolve the ground state of the antiferromagnetic Ising model (i.e. the zero momentum Néel state) with the anisotropic Heisenberg Hamiltonian (with anisotropy $\Delta \geq 1$). For this nontrivially interacting situation, an application of the first-principles-based quench-action method allows us to give an exact description of the postquench steady state in the thermodynamic limit.We show that a generalized Gibbs ensemble, implemented using all known local conserved charges, fails to reproduce the exact quench-action steady state and to correctly predict postquench equilibrium expectation values of physical observables. This is supported by numerical linked-cluster calculations within the diagonal ensemble in the thermodynamic limit.

TT 19.2 Mon 15:15 H 3010

Auxiliary master equation approach to nonequilibrium correlated impurities: a matrix product states treatment — •Antonius Dorda, Wolfgang von der Linden, and Enrico Arrigoni — Graz University of Technology, Graz, Austria

The auxiliary master equation approach [1,2] allows for a direct and efficient calculation of steady state properties of correlated impurity problems out of equilibrium, as is needed e.g. for nonequilibrium dynamical mean field theory [3]. The basic idea is to replace the original impurity problem by an auxiliary one, described by an open quantum system consisting of a finite number of bath sites embedded in a Markovian environment. The system dynamics are then described by a Lindblad equation, in which the different bath parameters are optimized by fitting the bath hybridization function in Keldysh space. Upon increasing the number of bath sites, the results can be systematically improved and the solution of the auxiliary system converges towards the exact one. A systematic study using a non-Hermitian Lanczos solver has been carried out [1] and a good agreement with reference values was found already for rather small system sizes. In order to further increase the accuracy, matrix product states are employed to address the interacting Lindblad problem, which enables one to consider larger system sizes.

[1] A. Dorda et al., Phys. Rev. B 89, 165105 (2014)
[2] E. Arrigoni et al., Phys. Rev. Lett. 110, 086403 (2013)
[3] J. K. Freericks et al., Phys. Rev. Lett. 97, 266408 (2006)

TT 19.3 Mon 15:30 H 3010

Wannier-Stark Resonances in the current characteristics of an one-dimensional tight-binding chain and graphene nanoribbons: The role of interactions and dissipation — •Jakob Neumayer, Enirco Arrigoni, and Wolfgang von der Linden — Institut für Theoretische Physik - Computational Physics, Technische Universität Graz, Österreich

Electronic transport investigations of an infinite one-dimensional tight-binding chain and infinitely long graphene nanoribbons are performed within the Wannier-Stark model, where a homogeneous electric field is applied along the overall structure to drive a current to flow. Dissipation is represented in a simplified way by coupled voltage probes (artificial fermion bath chains) instead of an explicit consideration of phonons, to prevent an occurrence of Bloch Oscillations within the infinite geometries. Cluster Perturbation Theory is used to allow for an effective inclusion of electron correlations into the considered model.

Appearing Wannier-Stark resonances in the steady-state current characteristics of the correlated one-dimensional chain and graphene nanoribbons demand for a comprehensive understanding of the physical transport processes within the Wannier-Stark model, which is gained by an investigation of the physical system in terms of occurring resonant tunnelling processes. A non-interacting one-dimensional model system with alternating on-site energies is presented in conclusion, reproducing the current characteristics of the correlated tight-binding chain and allowing for a thorough explanation of the found oscillatory current behaviour.

TT 19.4 Mon 15:45 H 3010

Dynamics after connecting two fermionic chains — •Jacopo Viti[1], Jean-Marie Stephan[1], Jerome Dubail[2], and Masud Haque[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden — [2]Universite de Lorraine, 34 Cours Léopold, 54000 Nancy, France

I will consider a simple out-of-equilibrium protocol: Two one-dimensional systems of free fermions are initially prepared at different densities and/or temperatures; they are then joined together and allowed to evolve unitarily. I will describe the time evolution of two-point correlation functions, discussing in particular their stationary value and the way the steady regime is attained. Particle and thermal currents will be also analyzed. A description in terms of the semi-classical Wigner function will be presented.

TT 19.5 Mon 16:00 H 3010

Real-time dynamics of energy currents in perturbed Heisenberg spin-1/2 chains — •Robin Steinigeweg[1], Jacek Herbrych[2], Jochen Gemmer[3], and Wolfram Brenig[1] — [1]Institute for Theoretical Physics, Technical University Braunschweig, Germany — [2]CCQCN, University of Crete, Greece — [3]Department of Physics, University Osnabrück, Germany

We use the concept of typicality to study the real-time dynamics of energy currents in nonintegrable spin-1/2 models in one dimension and at nonzero temperatures. These models are perturbed XXZ chains, where the integrability-breaking perturbation is either a staggered magnetic field or a complex exchange-coupling structure. Within linear response theory, we numerically calculate autocorrelation functions by propagating a single pure state, drawn at random as a typical representative of the full statistical ensemble. By comparing to small-system data from exact diagonalization and existing data from tDMRG, we show that typicality is satisfied in finite systems over a wide temperature range and valid in both, integrable and nonintegrable systems. We also confirm the validity of our approach by comparing to spectra from Lanczos diagonalization. For the large system sizes treatable, we observe little finite-size effects for large and small perturbation strengths. This allows us to obtain the full relaxation curve of the energy current and to determine the scaling of the heat conductivity.

[1] R. Steinigeweg, J. Gemmer, W. Brenig, PRL 112, 120601 (2014).
[2] R. Steinigeweg, J. Gemmer, W. Brenig, arXiv:1408.6837 (2014).
[3] R. Steinigeweg, J. Herbrych, W. Brenig, in preparation.

TT 19.6 Mon 16:15 H 3010

Dynamical Quantum Phase Transitions in the Kitaev Honeycomb Model — •Markus Schmitt and Stefan Kehrein — In-

stitut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

The notion of a dynamical quantum phase transition (DQPT) was recently introduced by Heyl et al. as the non-analytic behaviour of the dynamical free energy at critical times in the real time evolution of quantum systems in the thermodynamic limit [Heyl et al., Phys. Rev. Lett., 110:135704, 2013]. We present results for the quench dynamics in the vortex-free sector of the two-dimensional Kitaev honeycomb model, which can be mapped to BCS-form, regarding the occurrence of DQPTs. For general two-dimensional systems of BCS-type the zeros of the dynamical partition function coalesce to areas in the thermodynamic limit and DQPTs are of second order. In the Kitaev honeycomb model these DQPTs occur after quenches across a phase boundary or within the massless phase. Considering the 1d limit of the Kitaev honeycomb model it becomes clear that the higher order of the DQPTs is intimately related to the higher dimensionality of the non-degenerate model. Moreover, a conjectured connection between the appearance of DQPTs and ergodicity, which becomes manifest as a relation between the long time limit of the dynamical free energy and the fidelity, is found to hold for the Kitaev honeycomb model.

15 min. break.

TT 19.7 Mon 16:45 H 3010

Real-time dynamics of lattice bosons from nonequilibrium dynamical mean-field theory — •Hugo Strand[1], Martin Eckstein[2], and Philipp Werner[1] — [1]Department of Physics, University of Fribourg, Fribourg, Switzerland — [2]Max Planck Research Department for Structural Dynamics, University of Hamburg-CFEL, Hamburg, Germany

We extend bosonic dynamical mean-field theory to nonequilibrium situations in combination with a Nambu strong coupling impurity solver [1]. As a first application we study bosonic cold-atoms in an optical lattice using the Bose-Hubbard model and investigate the Mott insulating, superfluid and normal phases at finite temperatures. We perturb the system by quenching the interaction, mimicking the seminal experiment of Greiner et al. [2], and study its time-evolution. Starting from both the normal and superfluid phase, we map out nonequilibrium phase diagrams of the different dynamical regimes, such as rapid thermalization, and trapping in meta-stable normal and superfluid states. Depending on parameters, the condensate displays long lived or strongly damped amplitude oscillations. Nonequilibrium bosonic dynamical mean-field theory can directly be extended to nonequilibrium bosonic multi-component systems [3] and Bose-Fermi mixtures [4].

[1] HS, ME, PW arXiv:1405.6941.
[2] M. Greiner, O. Mandel, T. W. Hansch, I. Bloch, Nature 419, 51 (2002).
[3] A. Hubener, M. Snoek, W. Hofstetter, PRB 80, 245109 (2009).
[4] P. Anders, P. Werner, M. Troyer, M. Sigrist, L. Pollet, PRL 109, 206401 (2012).

TT 19.8 Mon 17:00 H 3010

Dynamical phase transitions in the mean field Ising model — •Ingo Homrighausen and Stefan Kehrein — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

The complexity of quantum many body physics leads to interesting phenomena far from equilibrium. An accessible quantity that characterizes the non-equilibrium quantum dynamics after a quantum quench is the return probability (Loschmidt echo). Dynamical phase transitions (DPTs) are defined as non-analyticities in the time-dependence of the return probability rate function in the thermodynamic limit. These DPTs were first observed in the one dimensional transverse-field Ising model for quenches across the quantum critical point [1]. Thereafter they have been studied mostly in low-dimensional exactly solvable models. We investigate the existence of DPTs in the infinite-dimensional mean field limit of the transverse-field Ising model. Now, in contrast to the one-dimensional case, DPTs occur for quenches across the equilibrium phase boundary as well as for quenches within the ordered phase. Moreover, in addition to the non-analytic behavior of the return probability we also find non-analyticities in the rate function of the work distribution for non-zero work. Based on a semi-classical analysis we explain the mechanism behind our findings.

[1] Heyl et al., Phys. Rev. Lett. 110, 135704 (2013)

TT 19.9 Mon 17:15 H 3010

Many-body localization and quantum ergodicity in disordered long-range Ising models — Philipp Hauke[1] and •Markus Heyl[2] — [1]Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria — [2]Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, 6020 Innsbruck, Austria

Ergodicity in quantum many-body systems is - despite its fundamental importance - still an open problem. Many-body localization provides a general framework for quantum ergodicity, and may therefore offer important insights. In this talk, it will be shown using both numerical and analytical methods that long-range interacting Ising models with transverse-field disorder enter a many-body localized phase at infinite temperature, irrespective of the disorder strength. As a consequence, these systems are nonergodic. To characterize and quantify quantum ergodicity, a measure for distances in Hilbert space will be introduced. It will be shown that in spin-1/2 systems it is equivalent to a simple local observable in real space, which can be measured in current experiments of superconducting qubits, polar molecules, Rydberg atoms, and trapped ions.

TT 19.10 Mon 17:30 H 3010

Statistical properties of all eigenstates in isolated quantum systems — •Wouter Beugeling, Alexei Andreanov, Roderich Moessner, and Masud Haque — Max-Planck-Institut für Physik komplexer Systeme (MPIPKS), Dresden, Germany

Traditionally, the focus of research in quantum many-body systems has been the ground state and low-lying excited states. For isolated quantum systems, however, the complete spectrum is relevant, because a mechanism that lets the system equilibrate to low energy is absent. The eigenstates in the bulk of the spectrum have significantly different properties than those at the edge, which shows for instance in the entanglement entropy, which typically follows a volume law in the bulk and an area law at the edge.

In this talk, I will discuss the typical behaviour of entanglement entropy and participation ratios of eigenstates as a function of location in the spectrum. Motivated by the similar behaviour of high values in the bulk and low values at the edge, and by the interpretation of both as measures of randomness in the eigenstates, we quantitatively analyse the correlation between the two quantities. We connect their behaviour to that of diagonal and off-diagonal matrix elements of local observables. To this end, we study the dependence on system size and on the amount of integrability breaking, which we introduce by looking at tunable Hamiltonians.

TT 19.11 Mon 17:45 H 3010

Real-time polaron formation: a nonequilibrium DMFT study — •Sharareh Sayyad and Martin Eckstein — Max Planck Research Department for Structural Dynamics, University of Hamburg-CFEL, Hamburg, Germany

To characterize the real-time polaron formation, we study the interaction-quench in the one-band Holstein model for the low density limit of carriers [1]. In this talk, first, we will briefly discuss the exact nonequilibrium self-energy within the framework of the dynamical mean field theory. Furthermore, we will describe the emergence of a polaron in the strong coupling limit, which is indicated by the splitting the band into the "dressed" electronic band as well as a dispersion-less "polaronic" one. Finally, we will investigate the properties of the real-time formed-polaron and compare them to their equilibrium counterparts.

[1] Sh. Sayyad, M. Eckstein, arXiv:1410.4298(2014).

TT 20: Transport: Topological Insulators 1 (jointly with DS, HL, MA, O)

Time: Monday 15:00–17:45 Location: A 053

Invited Talk TT 20.1 Mon 15:00 A 053

The Wires' Approach to Topological Insulators — •Yuval Oreg — Weizmann Institute of Science, Rehovot, Israel

We suggest a construction of a large class of topological states using an array of quantum wires. We will show how to construct a Chern insulator using an array of alternating wires that contain electrons and holes, correlated with an alternating magnetic field. A generalization to wires, with alternating spin-orbit couplings which give rise to integer and fractional (Abelian and non-Abelian) topological insulators, is then straightforward.

Following this construction we will discuss suggestions for two possible experiments which give rise to a fractional Josephson-effect and in addition a novel spin-resolved current correlation effect.

TT 20.2 Mon 15:30 A 053

Helical Majorana surface states of strongly disordered topological superconductors with time-reversal symmetry — •Raquel Queiroz and Andreas Schnyder — Max Planck Instutute for Solid State Research, Stuttgart, Germany

Noncentrosymmetric superconductors with strong spin-orbit coupling and the B phase of ^{3}He are possible realizations of topological superconductors with time-reversal symmetry. The nontrivial topology manifests itself at the material's surface in terms of linearly dispersive helical Majorana modes protected by symmetry from disorder weaker than the superconducting gap. Using extensive numerical simulations, we investigate the stability and properties of these Majorana states under strong surface disorder, which influences both bulk and surface states. A critical crossover from weak to strong disorder is observed in both two and three dimensions, through which an extended state exactly at zero energy always persists. The localization properties of the ingap states are studied through the distribution of the local density of states and level repulsion statistics.

TT 20.3 Mon 15:45 A 053

Intrinsic conduction through topological surface states of insulating Bi_2Te_3 epitaxial thin films — •Katharina Hoefer[1], Christoph Becker[1], Diana Rata[1], Jesse Swanson[1,2], Peter Thalmeier[1], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden — [2]University of British Columbia, Vancouver

Topological insulators represent a new state of matter that open up new opportunities to create unique quantum particles. Many exciting experiments have been proposed by theory, yet, the main obstacle for their execution is material quality and cleanliness of the experimental conditions. The presence of tiny amounts of defects in the bulk or contaminants at the surface already mask these phenomena.

We present the preparation, structural and spectroscopic characterisation of MBE-grown Bi_2Te_3 thin films that are insulating in the bulk. Moreover, temperature dependent four-point-probe resistivity measurements of the Dirac states on surfaces that are intrinsically clean were conducted. The total amount of surface charge carries is in the order of $10^{12}\,\mathrm{cm}^{-2}$ and mobilities up to $4600\,\mathrm{cm}^2/\mathrm{Vs}$ are observed.

Importantly, these results are achieved by carrying out the preparation and characterisation all in-situ under ultra-high-vacuum conditions [1].

[1] K. Hoefer et al. PNAS, 2014, 111(42), 14979-14984.

TT 20.4 Mon 16:00 A 053

Quantum interference of edge supercurrents in a two-dimensional topological insulator — •Grigory Tkachov, Pablo Burset, Björn Trauzettel, and Ewelina Hankiewicz — Würzburg University

Josephson weak links made of two-dimensional topological insulators (TIs) exhibit magnetic oscillations of the supercurrent that are reminiscent of those in superconducting quantum interference devices (SQUIDs). We propose a microscopic theory of such a TI SQUID effect [1]. The key ingredient of our model is the exact treatment of the influence of an external magnetic field on the edge supercurrents. We show that this influence has the form of a 1D Doppler effect that describes the flux-controlled interference of the edge currents with superimposed suppression of Andreev reflection. Both long and short junctions are discussed. In particular, for long junctions the theory shows a temperature-driven crossover from the normal Φ_0-periodic SQUID pattern to a $2\Phi_0$-quasiperiodic pattern consisting of a series of alternating even and odd peaks (where $\Phi_0 = ch/2e$ is the magnetic flux quantum). The predicted even-odd effect is the signature of gapless (protected) Andreev bound states with a sawtooth dependence on the magnetic flux. Our findings may shed some light on the recently observed even-odd interference pattern in InAs/GaSb-based TI Josephson junctions, suggesting new operation regimes for nano-SQUIDs.

[1] G. Tkachov, P. Burset, B. Trauzettel, and E. M. Hankiewicz, arXiv:1409.7301.

TT 20.5 Mon 16:15 A 053

Rashba spin-orbit coupling at the quantum spin Hall edge — •Florian Geissler, Francois Crepin, and Björn Trauzettel — Universität Würzburg, Institut für Theoretische Physik und Astrophysik, Germany

Not only since the discovery of the quantum spin Hall effect, and up to most recent questions in the context of topological insulating materials, transport through one-dimensional systems is a problem of great importance and interest. In a quantum spin Hall system, electron transport occurs in conducting edge channels, that are spin-filtered with respect to their direction of motion, and was shown to be topologically protected by time-reversal symmetry. We use the helical Luttinger liquid model to study transport in such systems, when the perfect conductance is perturbed. Particularly, we show that a potential source of backscattering is provided by the combination of a Rashba spin-orbit coupling (SOC) impurity and electron-electron interactions, even though time-reversal symmetry remains preserved. Based on both renormalization group and Keldysh calculations, the scaling of the conductance with the external bias is derived at zero temperature. Moreover, we illustrate, that such SOC-impurities may give rise to interesting effects when being present in an interface of a Luttinger liquid connected to a superconductor.

15 min. break.

TT 20.6 Mon 16:45 A 053

Coexisting edge states and gapless bulk in topological states of matter — Yuval Baum[1], •Thore Posske[2], Ion Cosma Fulga[1], Björn Trauzettel[2], and Ady Stern[1] — [1]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We consider two dimensional systems in which edge states coexist with a gapless bulk. Such systems may be constructed, for example, by coupling a gapped two dimensional state of matter that carries edge states to a gapless two dimensional system in which the spectrum is composed of a number of Dirac cones. We find that in the absence of disorder the edge states could be protected even when the two systems are coupled, due to momentum and energy conservation. We distinguish between weak and strong edge states by the level of their mixing with the bulk. In the presence of disorder, the edge states may be stabilized when the bulk is localized or destabilized when the bulk is metallic. We analyze the conditions under which these two cases occur. Finally, we propose a concrete physical realization for one of our models on the basis of bilayer Hg(Cd)Te quantum wells.

TT 20.7 Mon 17:00 A 053

Spin texture of generic helical edge states — •Alexia Rod[1], Thomas L. Schmidt[2], and Stephan Rachel[1] — [1]Institut für Theoretische Physik, TU Dresden, Germany — [2]Department of Physics, University of Basel, Switzerland

Edge states of time-reversal topological insulators can be described as helical Luttinger liquids. The generic helical liquid is the most general model of a time-reversal invariant helical liquid without axial spin symmetry. This symmetry is usually broken in experimental realizations, and it has been shown that its absence changes the transport properties significantly [1]. For a translation invariant system, the breaking of axial spin symmetry manifests itself in a momentum-dependent rotation of the spin quantization axis. Its manifestation in real space has remained, however, elusive so far.

Here we show that one can extract the rotation of spin quantization axis also in real space, e.g. for topological insulator disks with broken spin symmetry but also other geometries which are not rotationally invariant [2]. This suggests that the concept of a generic helical liquid is independent of the microscopic model and the considered geometry.

[1] T.L. Schmidt, S. Rachel, F. von Oppen, L. Glazman, Phys. Rev. Lett. 108, (2012).
[2] A. Rod, T.L. Schmidt, S. Rachel, manuscript in preparation.

TT 20.8 Mon 17:15 A 053

Manipulation of helical edge state transport by a quantum magnet — •Peter Silvestrov[1], Patrik Recher[1], and Piet Brouwer[2] — [1]Institute for Mathematical Physics, TU Braunschweig — [2]Dahlem Center for Complex Quantum Systems, FU Berlin

Application of a magnetic field is usually considered as a way to open the gap in the spectrum of helical edge states, leading to a blocking of the edge current. Nevertheless, it was shown recently that the current is fully transmitted through the gapped region in case of interaction with a quantum magnet[1]. Here we consider other interesting features of the helical edge state current interacting with the magnet. First, we notice that although the current is transmitted, all electrons with energies close to the Fermi energy are fully reflected. The actual current is carried by the electrons with energies below the gap and well below the Fermi energy. This suggests that the magnet while allowing passing the current, fully blocks the thermal transport thereby acting as a cooler for the injected electron beam. Our second setup consists of two helical edges covered by the same magnet. The current injected into one edge creates a non-equilibrium magnetization driving a current in the second edge. The current in the first edge is now half-reflected and half-transmitted by the magnet. However, the partial reflection of the current does not cause any shot noise.

[1] Q.Meng, S.Vishveshwara, T.L.Hughes, arXiv:1312.7303.

TT 20.9 Mon 17:30 A 053

Probing spin-polarized edge state superconductivity by Andreev reflection in in-plane magnetic fields — •Rolf W. Reinthaler, Grigory Tkachov, and Ewelina M. Hankiewicz — Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany

Finding signatures of unconventional superconductivity in Quantum Spin Hall systems is one of the challenges of solid state physics. Here we induce superconductivity in a 3D topological insulator thin film to cause the formation of helical edge states, which are protected against backscattering even in finite magnetic fields. Above a critical in-plane magnetic field, which is much smaller than the critical field of typical superconductors, the quasi-particle gap closes, giving rise to energy-dependent spin polarization. In this regime the spin-polarized edge state superconductivity can be detected by Andreev reflection. We propose measurement setups to experimentally observe the spin-dependent excess current and dI/dV characteristics.

TT 21: Superconductivity: Poster Session

Time: Monday 15:00–18:00 Location: Poster B

TT 21.1 Mon 15:00 Poster B

Pinning centres in ISD-MgO coated conductors — •Benjamin H. Stafford[1,2], Oleksiy Troshyn[1], Jens Hänisch[3], Rueben Hühne[2], Veit Grosse[1], Markus Bauer[1], Werner Prusseit[1], Bernhard Holzapfel[3], and Ludwig Schultz[2] — [1]THEVA Dünnschichttechnik GmbH, Rote-Kreuz-Str. 8, D-85737 Ismaning, Germany — [2]Institute for Metallic Materials, IFW Dresden, PO Box 27 01 16, D-01171 Dresden, Germany — [3]Institute for Technical Physics, Karlsruhe Institute of Technology (KIT), PO Box 36 40, D-76021 Karlsruhe, Germany

High temperature superconductor (HTS) films on long length metallic tapes, known as coated conductors, are quickly becoming a reality for use in superconducting motors and generators. One way to ensure good biaxial texturing of the HTS film is via the use of a buffer layer deposited by inclined substrate deposition (ISD). In order to improve the in-field performance of such coated conductors, nanoscale inclusions can be incorporated into the HTS layer to pin flux vortices. Until now it is not known how effectively such pinning centres can be incorporated into HTS films grown on ISD substrates due to the unique growth process of the HTS layer. In this work we have prepared $GdBa_2Cu_3O_{7-x}$ films grown heteroepitaxially on ISD-MgO buffered tapes via e-beam evaporation. We show how such nanoscale inclusions are arranged within the film. We also present data for the in-field critical current anisotropy of such films, displaying the effectiveness of the incorporated inclusions as pinning centres.

TT 21.2 Mon 15:00 Poster B

Leggett modes in superconductors without inversion symmetry — •Nikolaj Bittner[1], Dietrich Einzel[2], Ludwig Klam[1], and Dirk Manske[1] — [1]Max–Planck–Institut für Festkörperforschung, D–70569 Stuttgart, Germany — [2]Walther–Meißner–Institut für Tieftemperaturforschung, D–85748 Garching, Germany

The recent discovery of bulk superconductors without inversion symmetry has allowed for a new understanding of pairing correlations in general. These so–called non–centorsymmetric superconductors (NCS) are characterized by the existence of an antisymmetric spin–orbit coupling. As a consequence, there occurs a band splitting, accompanied with the coexistence of both singlet and triplet contributions to the superconducting gap. The band splitting implies the existence of a new massive collective mode, which was discovered by A. J. Leggett in 1966 for ordinary two–band superconductors, the so–called Leggett mode. Within the framework of the (Nambu) Matrix Kinetic Theory we show, that (i) in contrast to the case of the ordinary two–band superconductors, where the Leggett mode appears always as a massive collective excitation, its counterpart in NCS systems can be massless under certain conditions, (ii) it survives in the limit of vanishing triplet admixture $t = \Delta_{tr}/\Delta_s$ to the singlet energy gap and (iii) Anderson–Higgs mechanism leaves its mass unaffected.

TT 21.3 Mon 15:00 Poster B

Signatures of the nonequilibrium dynamics of superconductors in the pump-probe response — •Holger Krull[1], Götz S. Uhrig[2], Andreas P. Schnyder[1], and Dirk Manske[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]TU Dortmund, Dortmund, Germany

We present theoretical studies of the pump-probe response of nonequilibrium superconductors coupled to optical phonons. Considering ultra-short pump pulses, the superconductor is pushed into the nonadiabatic regime. It is characterized by oscillations of the order parameter as well as by the generation of coherent phonons. Using the density matrix formalism, we compute the pump-probe response and determine signatures of the order parameter and of the phonon dynamics in the pump-probe conductivity. We find that the nonadiabatic dynamics of the superconductor is reflected in the oscillation in the conductivity as function of the delay time between pump and probe pulse.

TT 21.4 Mon 15:00 Poster B

Large Oscillations of the Magnetoresistance in Nanopatterned Thin Aluminum Films — •Christopher Espy[1], Julian Braun[1], Benjamin Lindner[1], Omri Sharon[2], Elke Scheer[1], and Yosef Yeshurun[2] — [1]Universität Konstanz, Konstanz, Germany — [2]Bar-Ilan University, Ramat Gan, Israel

With their experiments on thin superconducting cylinders Little and Parks demonstrated oscillations of the critical temperature with the flux threading the cylinder [1]. The periodicity of $\Phi_0 = h/2e$ supported the picture of a correlated two-electron state, as predicted by BCS theory. However, theoretical studies predict a h/e periodicity in ring-shaped unconventional superconductors that can arise via various mechanisms, when the ring diameter becomes comparable to the coherence length, ξ_0 [2, 3].

There is even speculation that this periodicity should be seen in rings made out of aluminum, a conventional s-wave superconductor, with diameters smaller than the coherence length, i.e. in the order of 1 μm [3]. Sochnikov et al. investigated this proposed periodicity in double network patterns of $La_{1.84}Sr_{0.16}CuO_4$ but did not find the predicted periodicity [4]. We show first results of our experiments on such double networks of aluminum nano-rings.

[1] Little, W.A. and Parks, R. D., PRL 9, 9 (1962).

[2] Vakaryuk, V., PRL 101, 167002 (2008).
[3] Loder, F. et al., PRB 78, 174526 (2008).
[4] Socknikov, I. et al., Nat. Nanotech. 5, 516 (2010).

TT 21.5 Mon 15:00 Poster B

Superconducting NbN single-photon detectors on GaAs with an AlN buffer layer — •Ekkehart Schmidt, Michael Merker, Konstantin Ilin, and Michael Siegel — Institut für Mikro- und Nanoelektronische Systeme (IMS), Karlsruher Institut für Technologie, Hertzstrasse 16, 76187 Karlsruhe, Deutschland

GaAs is the material of choice for photonic integrated circuits. It allows the monolithic integration of single-photon sources like quantum dots, waveguide based optical circuits and detectors like superconducting nanowire single-photon detectors (SNSPDs) onto one chip. The growth of high quality NbN films on GaAs is challenging, due to natural occurring surface oxides and the large lattice mismatch of about 27%. In this work, we try to overcome these problems by the introduction of a 10 nm AlN buffer layer. Due to the buffer layer, the critical temperature of 6 nm thick NbN films was increased by about 1.5 K. Furthermore, the critical current density at 4.2 K of NbN flim deposited onto GaAs with AlN buffer is 50% higher than of NbN film deposited directly onto GaAs substrate. We successfully fabricated NbN SNSPDs on GaAs with a AlN buffer layer. SNSPDs were patterned using electron-beam lithography and reactive-ion etching techniques. Results on the study of detection efficiency and jitter of a NbN SNSPD on GaAs, with and without AlN buffer layer will be presented and discussed.

TT 21.6 Mon 15:00 Poster B

THz Spectroscopy on Superconducting NbN Thin Films — •Lena Daschke[1], Uwe S. Pracht[1], Martin Dressel[1], Marc Scheffler[1], Konstantin S. Ilin[2], and Michael Siegel[2] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Institut für Mikro- und Nanoelektronische Systeme, Karlsruher Institut für Technologie

Epitaxial thin-film niobium nitride (NbN) is a conventional BCS superconductor. In presence of strong disorder, however, electronic inhomogeneities appear, which is not fully understood yet. To obtain a better insight into the physics of such disordered materials, studies on model systems such as structurally tailored films might be useful. Furthermore, disordered NbN films are used for single-photon detection devices, whose proper performance depends on a profound understanding of the superconducting properties. The studied NbN films have a T_c ranging from 10 to 15 K and the superconducting energy gap is easily accessible with THz spectroscopy (0.4 - 5.6 meV).

We investigate thin films of NbN sputtered on a sapphire substrate. With a Mach-Zehnder interferometer we measure the amplitude and phase shift of radiation transmitted through the thin-film sample. From there we can determine the real and imaginary parts of the optical conductivity. These results give information about the energy gap, Cooper pair density, and quasiparticle dynamics, including the temperature evolution of these quantities. We found that a film with 10 nm thickness roughly follows the BCS behavior, as expected. We will present results of our measurements on several different NbN samples.

TT 21.7 Mon 15:00 Poster B

Reduction of current-crowding effect in bended superconducting structures — •Ilya Charaev, Konstantin Ilin, and Michael Siegel — Institut für Mikro- und Nanoelektronische Systeme, Karlsruhe Institut für Technologie (KIT), Hertzstraße 16, 76187 Karlsruhe, Germany

Suppression of critical current Ic in superconducting structures with defects belongs to one of fundamental problems of superconductivity. One of mechanisms of suppression of Ic is a current-crowding effect, i.e. increase of current density in vicinity of defect. Detailed analysis of current-crowding effect in mesoscopic superconducting structures has been done by Clem in [1]. We demonstrate increase of the critical current of superconducting nanowires by an external magnetic field which is applied normally to the structure surface. The critical current of single-spiral nanowires with sharp bends, which play a role of artificially created defects, is 20% higher in magnetic field B = 25 mT than Ic of the same structure at B = 0 T. In case of single-spiral nanowires without sharp bends, the difference between Ic in magnetic field and Ic at B = 0 T was 5% only in good agreement with theoretical predictions. A detailed analysis of the influence of the magnetic field on transport properties of superconducting mesoscopic structures with artificial defects will be presented and discussed in terms of possible application of this effect for improvement of performance of superconducting nanowire single-photon detector.

TT 21.8 Mon 15:00 Poster B

Superconductivity in the ferecrystals $[(SnSe)_{1+\delta}]_m(NbSe_2)_1$ — •Corinna Grosse[1], Matti Alemayehu[2], Georg Hoffmann[1], Andreas Fiedler[1], Olivio Chiatti[1], Anna Mogilatenko[1,3], David C. Johnson[2], and Saskia F. Fischer[1] — [1]Novel Materials, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Chemistry, University of Oregon, Eugene, OR, 97401, USA — [3]Ferdinand-Braun-Institut, Leibniz-Institut fürHöchstfrequenztechnik, 12489 Berlin, Germany

The ferecrystals $[(SnSe)_{1+\delta}]_m(NbSe_2)_1$ are novel layered materials consisting of single-layer $NbSe_2$ sheets alternately stacked with m double layers of SnSe. $NbSe_2$ exhibits interesting electrical properties such as charge density waves and superconductivity. In contrast to conventional misfit layer compounds, ferecrystals are turbostratically disordered and the individual layer thicknesses are tunable.

We investigate the structural and electrical properties of the ferecrystals $[(SnSe)_{1+\delta}]_m(NbSe_2)_1$. The crystal structure was analyzed using scanning transmission electron microscopy, visualizing the ferecrystal layer structure on the atomic scale. The ferecrystals were characterized by measuring in-plane resistivity, magnetoresistance and Hall coefficients. A superconducting transition was observed in the resistivity measurements. The transition temperatures and the in-plane and cross-plane coherence lengths were investigated as a function of the thickness of the SnSe layers, which separate the $NbSe_2$ single-layers. The relationship between the coherence lengths and the atomic structure of these quasi-two-dimensional materials is discussed.

TT 21.9 Mon 15:00 Poster B

Superconductivity and ferromagnetism in nanostructured Bi_3Ni — •R. Schönemann[1], T. Herrmannsdörfer[1], H. Kühne[1], Z. Zhang[1], M. Naumann[1], R. Skrotzki[1,2], M. Kaiser[2], M. Heise[2], M. Ruck[2], K. Kummer[3], D. Graf[4], and J. Wosnitza[1] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Chemistry and Food Chemistry, TU Dresden, Dresden, Germany — [3]European Synchrotron Radiation Facility (ESRF), Grenoble, France — [4]National High Magnetic Field Laboratory and Department of Physics, Florida State University, Tallahassee, Florida, USA

We have demonstrated the coexistence of superconductivity and ferromagnetism in Bi_3Ni nanostructures which have been prepared by making use of novel chemical-reaction paths [1]. Here, we present recent experiments on new nanostructures, such as supercrystals consisting of packed Bi_3Ni nanofibers. We have investigated their structural, magnetic and electrical-transport properties by means of NMR, XMCD, SQUID magnetometry and ac-resistance measurements. In agreement with x-ray diffraction experiments, the ^{209}Bi NMR spectra indicate a distribution of local structural parameters in the Bi_3Ni nano fibres. While bulk Bi_3Ni is nonmagnetic, XMCD measurements on nanostructured Bi_3Ni indicate a magnetic $3d^8$ configuration of Ni. Resistivity measurements demonstrate that superconductivity persists well above the Pauli limiting field - with strong anisotropy.

[1] T. Herrmannsdörfer, R. Skrotzki, J. Wosnitza, D. Köhler, R. Boldt, M. Ruck, Phys. Rev. B 83, 140501 (R) (2011).

TT 21.10 Mon 15:00 Poster B

Superconductivity in the unconventional high pressure phase bismuth-III — •Konstantin Semeniuk, Philip Brown, Aleksandar Vasiljkovic, and Malte Grosche — University of Cambridge, Cambrige, The United Kingdom

One of the most surprising developments in high pressure research was the realisation that many elements assume very unexpected high pressure structures, described in terms of extremely large or even infinite unit cells. Elemental bismuth, which has been known to undergo a series of pressure induced structural transitions between 25 kbar and 80 kbar, is an interesting example: the intermediate pressure Bi-III phase has a complex 'host-guest' structure consisting of two incommensurate sublattices. Since the unit cell is infinitely large, the description of electronic and lattice excitations is problematic. Apart from its metallic character and the observation of superconductivity at low temperature, little is known about the electronic structure in this phase.

We investigate the electrical resistivity within the metallic Bi-III phase under high hydrostatic pressure and in applied magnetic field using a piston cylinder cell. Superconductivity is observed below 7.1 K, and we extract the temperature dependence of the upper critical

field, which exceeds 2 T at low temperature. The normal state resistivity exhibits an approximately linear temperature dependence. This could be attributed to strong scattering from low-lying excitations, as caused by an unusually soft phonon spectrum. The results suggest that strong coupling superconductivity arises within the host-guest structure of Bi-III out of an unusual electronic state.

TT 21.11 Mon 15:00 Poster B

Antimony Substitution in SmFeAsO — •Daniel Schmidt and Hans F. Braun — Universität Bayreuth

In the iron based compounds structural and magnetic phase transitions can be suppressed by applying external hydrostatic pressure and superconductivity emerges. Beside hydrostatic pressure, it is possible to apply chemical pressure by the substitution of atoms in the compounds with smaller ones. Such a substitution was successful for example in $LaFeAs_{1-x}P_xO$, where the parent compound shows a structural and a spin-density-wave transition and the P doped samples become superconducting. We are interested in the opposite way and substitute the As by the bigger Sb. In literature, the substitution in the La-1111 compounds was possible up to a substitution level of 40 %. With Sm, instead of La, we used a smaller rare-earth metal. We present the results obtained on polycrystalline samples characterized by Xray powder diffraction and resistivity measurements.

TT 21.12 Mon 15:00 Poster B

Impact of Y and Mn-codoping on magnetism and superconductivity in $La_{1-z}Y_zFe_{1-y}Mn_yAsO_{1-x}F_x$ — •Rhea Kappenberger[1], Franziska Hammerath[1,2,3], Mesfin Asfaw Afrassa[1,4], Pietro Carretta[2], Samuele Sanna[2], Rowena Wachtel[1], Christian G.F. Blum[1], Anja Wolter-Giraud[1], Sabine Wurmehl[1,3], and Bernd Büchner[1,3] — [1]IFW Dresden, Institute for Solid State Research, D-01171 Dresden, Germany — [2]Dipartimento di Fisica and Unitá di CNISM di Pavia, Pavia, Italy — [3]Institut für Festkörperphysik, TU Dresden, Dresden, Germany — [4]Addis Ababa University, Addis Ababa, Ethiopia

It has been shown by Kamihara et al. [1] that F doping of the iron oxypnictide LaFeAsO leads to the emergence of superconductivity. Doping of the parent compound with Y on the La site also increases T_c [2], whereas Mn doping on the Fe site has been reported to have a detrimental effect to superconductivity [3,4]. We investigated the interplay of doping by substituting those different positions at the same time. The samples where characterized using EDX, XRD, SQUID and μSR. It was shown that Y doping indeed has a stabilizing effect on the superconductivity even in the presence of small amounts of Mn.

[1] Y. Kamihara et al., J. Am. Chem. Soc. 130, 3296 (2008).
[2] H. Takahashi, K. Igawa, K. Arii, Y. Kamihara, M. Hirano, and H. Hosono, Nature London 453, 376 (2008).
[3] D. Berardan, L. Pinsard-Gaudart, and N. Drago, J. Alloys Compd. 481, 470 (2009).
[4] F. Hammerath et al., Phys. Rev. B 89, 134503 (2014).

TT 21.13 Mon 15:00 Poster B

Observation of the Josephson effect on Ba-122 iron pnictide single crystals — •Noor Hasan[1], Stefan Schmidt[1], Sebastian Döring[1], Volker Tympel[1], Frank Schmidl[1], Paul Seidel[1], and Thomas Wolf[2] — [1]Friedrich-Schiller- Universität Jena , Institut für Festkörperphysik , Helmholtzweg 5, 07743 Jena, Germany — [2]Karlsruhe Institute of Technology, Institut für Festkörperphysik , Hermann-von- Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Since the discovery of the first Fe-based superconductors in 2006, extensive effort has been directed characterizing and modeling the novel properties of these exotic materials. Therefore Josephson junction offer ways to investigate the fundamental properties of iron pnictides. We use $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals, prepared by a self-flux method , with an optimal Co concentration of 0.065 (critical temperature T_c=23.5K) . We realize Josephson junctions along the c-axis. To prepare them a newly developed surface polishing as well as standard thin film technologies are used. The artificial barrier consists of thin sputtered layers of various materials, normal conductors as well as insulators. A thermally evaporated double layer film of Pb and In was used as the counter electrode. For the characterization of the Josephson effect we will present temperature dependent I-V characteristics as well as $I_cR_n - T$ dependencies and measurements under microwave radiation, including. Additionally results from tunneling and Andreev spectroscopy i.e temperature dependent dI/dV - V spectra are shown.

TT 21.14 Mon 15:00 Poster B

Pressure and field dependence of superconductivity in $RbFe_2As_2$ — •Pascal Reiss[1], Konstantin Semeniuk[1], Philip Brown[1], Kai Grube[2], Thomas Wolf[2], Peter Adelmann[2], Hilbert von Löhneysen[2], and F Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76131 Karlsruhe, Deutschland

$RbFe_2As_2$ is a member of the extensively investigated family of 122 iron based superconductors AFe_2As_2. It acts as the link between A=K and Cs, and as extremal hole-doping for A=Sr and Ba. The nature of the superconducting state in these compounds is still open, but likely to feature different nodal gap structures.

We report resistivity measurements of very pure (RRR > 1000) crystals of $RbFe_2As_2$. Superconductivity at ambient pressure and zero field is observed below 2.8K. We follow this transition and the upper critical field as a function of hydrostatic pressure up to 30 kbar.

Furthermore we observe a non-Fermi liquid form for the temperature dependence of the resistivity in the normal state, which we track as a function of pressure and applied magnetic field.

TT 21.15 Mon 15:00 Poster B

Electronic correlations in the superconductors AFe_2As_2 with A = K, Rb, and Cs — •Kai Grube[1], Felix Eilers[1], Diego A. Zocco[1], Peter Schweiss[1], Rolf Heid[1], Thomas Wolf[1], and Hilbert von Löhneysen[1,2] — [1]Karlsruhe Institute of Technology, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruhe Institute of Technology, Physikalisches Institut, 76131 Karlsruhe, Germany

Superconductivity in iron pnictides and chalcogenides occurs in the proximity to antiferromagnetic order, giving rise to the assumption that the superconductivity is unconventional and originates from electron-electron interactions. So far, experimental and theoretical studies underpin this assumption but fail to unravel the pairing mechanism. A central question is the role of electronic correlations in these materials. We have investigated the thermal expansion and magnetostriction of the stoichiometric compounds AFe_2As_2 with A = K, Rb, and Cs. Our measurements show a huge increase of the effective mass quasiparticles m_{eff} with increasing A ion radius, while the superconducting transition temperature T_c decreases. The relation between superconductivity and electronic correlations will be discussed by using the uniaxial pressure dependences of T_c and m_{eff} and the temperature dependence of the upper critical field.

TT 21.16 Mon 15:00 Poster B

Phase diagram of Fe-substituted $BaNi_2As_2$ — •Liran Wang[1], Anna Böhmer[1,2], Frédéric Hardy[1], Peter Schweiss[1], Thomas Wolf[1], and Christoph Meingast[1] — [1]Institute für Festkörperphysik,Karlsruher Institut für Technologie (KIT), 76344 Karlsruhe, Germany — [2]Department of Physics and Astronomy and Ames Laboratory, Iowa State University, Ames, Iowa 50011, USA

Recently, the phosphorus doped $BaNi_2As_2$[1] system was found to exhibit a large increase of T_c upon suppression of the structural transition, which was attributed to a large phonon softening at the critical concentration[2]. Here, we investigate the closely related $Ba(Ni_{1-2}Fe_x)_2As_2$ system, mostly on the iron-rich side, using high-resolution thermal expansion, specific heat, magnetization and resistivity measurements. We find a very similar suppression of the structural transition with Fe- as with P-doping, but do not find an enhanced superconducting transition. However, both the thermal expansion and resistivity exhibit anomalously large anomalies around the critical doping region, which are shown to be of non phononic origin. We discuss similarities and differences between both Fe- and P-substituted systems.

[1] N. Kurita et al., Phys. Rev. Lett. 102, 147004 (2009).
[2] K. Kudo et al., Phys. Rev. Lett. 109, 097002 (2012).

TT 21.17 Mon 15:00 Poster B

Optical measurements on iron pnictides containing Eu — •David Neubauer[1], Andreas Baumgartner[1], Johannes Merz[1], Sina Zapf[1], Saicharan Aswartham[2], Sabine Wurmehl[3], Wen-He Jiao[4], Guang-Han Cao[4], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]University of Kentucky, Lexington, USA — [3]IFW, Dresden, Germany — [4]Zhejiang University, Hangzhou, China

The interplay of magnetism with superconductivity is a fascinating,

highly debated field of research and many questions still remain unsolved. Members of the $EuFe_2As_2$ family are a perfectly suited playground for investigations concerning this topic, due to the peculiarity of strong local magnetism of the europium ($T_N \approx 20K$), which is a unique feature among the 122 iron pnictides. Optical studies of the parent compound have already revealed that the spin density wave formation deviates from the other 122 pnictides [1]. To get more insight into the superconducting properties of the $EuFe_2As_2$ family we carried out an optical study on differently doped samples. We compare $Eu(Fe_{1-x}Ir_x)_2As_2$ where electron doping takes place directly in the conducting iron layer, with $EuFe_2(As_{1-x}P_x)_2$ which corresponds to isovalent substitution at atomic positions out of the Fe-plane. The influence of the Eu is furthermore investigated by placing data we obtained on $Ba_{0.6}Eu_{0.4}(Fe_{1-x}Co_x)_2As_2$ in juxtaposition to the already highly investigated pure Ba analogue.

[1] D. Wu *et al.*, Phys. Rev. B **79**, 155103 (2009).

TT 21.18 Mon 15:00 Poster B

Persistent detwinning of $EuFe_2As_2$ by small magnetic fields — •Jannis Maiwald[1], Christian Stingl[1], Sina Zapf[2], Shuai Jiang[2], Nora Bach[1], Kirk Post[3], H. S. Jeevan[1], David Neubauer[2], Anja Löhle[2], Conrad Clauss[2], Dimitri Basov[3], Martin Dressel[2], and Philipp Gegenwart[1] — [1]Experimentalphysik VI, Universität Augsburg, Germany — [2]1.Physikalisches Institut, Universität Stuttgart, Germany — [3]Department of Physics, UC San Diego, USA

The formation of twin domains in the orthorhombic phase of high-temperature superconductors is impeding the investigation of the in-plane anisotropy of these materials. Recently, we have shown how the brief application of a small magnetic field of ~ 1 Tesla in the $EuFe_2As_2$ iron pnictide leads to a substantial detwinning of the system, which is persistent up to the structural transition at ~ 190 K even after the magnetic field has been switched off. This offers researchers the opportunity to investigate the detwinned iron arsenide without the application of any external symmetry breaking force, like the pressure of a mechanical clamp, or a magnetic field present during measurement. We will present angular dependent magnetoresistance, magnetostriction, thermal expansion and thermoelectric power measurements on the $EuFe_2As_2$ parent compound as well as on various doped variants in order to shed further light on the mechanism behind the field induced detwinning, i.e. the interplay of the involved magnetic moments stemming form the Eu and Fe atoms in these compounds.

TT 21.19 Mon 15:00 Poster B

Phase diagrams of $Ca(Fe,Ru)_2As_2$ system — •Kan Zhao and Philipp Gegenwart — Experimentalphysik VI, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

Single crystalline $Ca(Fe,Ru)_2As_2$ series have been grown and characterized by structural, magnetic, and transport measurements. These measurement shows $Ca(Fe,Ru)_2As_2$ undergoes successive phase transitions with increasing Ru element doping. The antiferromagnetic phase with orthorhombic structure at $x<0.023$ (x means the doping concentration of Ru element) is directly driven to a Fermi-liquid type collapsed tetragonal (cT) phase at $0.023<x<0.07$, with no superconducting region between the two phase, consistent with the conclusion of $CaFe_2As_2$ under hydrostatic pressure.

TT 21.20 Mon 15:00 Poster B

Pressure-induced superconductivity in $BaFe_2As_2$: optical study — •Ece Uykur[1], Tatsuya Kobayashi[2], Wataru Hirata[2], Shigeki Miyasaka[2], Setsuko Tajima[2], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, D-86195 Augsburg, Germany — [2]Department of Physics, Graduate School of Science, Osaka University, Osaka 560-0043, Japan

In previous studies, the superconductivity that arises from the antiferromagnetic state with various carrier dopings in iron-pnictide superconductors was demonstrated. Moreover, the external pressure induced superconductivity was shown by transport measurements. External pressure is a clean way to induce superconductivity compared to impurity doping cases. Moreover, it does not introduce additional carriers to the system. In this study, we performed temperature-dependent reflectivity measurements in $BaFe_2As_2$ parent compound under pressure (up to 5 GPa). At temperatures above the magnetic phase transition, the metallicity of the system is increasing with pressure. At lower temperatures, with increasing pressure the partial suppression of the magnetically ordered (SDW) state and the appearance of the superconducting (SC) state is observed at 3.6 and 4.2 GPa. At these pressures the SDW state and the SC state coexist. Moreover, the SC gap shows a full gap tendency below ~ 95 cm^{-1}.

TT 21.21 Mon 15:00 Poster B

Scanning tunneling microscopy study on $CaFe_2As_2$ surface — •Philipp Ansorg[1], Philip Willke[1], Kalobaran Maiti[2], Neeraj Kumar[2], Sudesh Kumar Dhar[2], Arumugum Thamizhavel[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Tata Institute of Fundamental Research Homi Bhabha Road, Colaba Mumbai-400 005, India

The discovery of high temperature superconductivity in cuprates leads to a great interest to examine also Fe-based systems. Superconductivity in the pnictide $CaFe_2As_2$ as a parent compound is induced by pressure or substitution of Fe by Co, Ni or other dopants.[1] Here we investigate the surface of $CaFe_2As_2$ by scanning tunneling microscopy and spectroscopy. Therefore the crystal [2] is cleaved under UHV conditions and cooled below the structural transition temperature of $T_S \approx 173$K by LN_2 or LHe. As found in similar systems [3] our STM data indicates a 2×1 surface reconstruction in the Ca layer at temperatures of both 6K and 77K. Furthermore anti-phase boundaries [4] along the 2×1 reconstruction can be observed.

[1] Y. Kamihara et al., J. Am. Chem. Soc. 128, 10012 (2006)
[2] G. Adhikary et al., J. Appl. Phys. 115, 123901 (2014)
[3] B. Saparov et al., Scientific Reports 4, 4120 (2014)
[4] K. Löser et al., Phys. Rev. B, 86, p. 085303 (2012)

TT 21.22 Mon 15:00 Poster B

High energy spectra on Fe-based unconventional superconductors — •Pranab Kumar Nag[1], Danny Baumann[1], Ronny Schlegel[1], Robert Beck[1], Sabine Wurmehl[1,2], Thomas Wolf[3], Bernd Büchner[1,2], and Christian Hess[1] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01171 Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, D-01062 Dresden, Germany — [3]Karlsruher Institut für Technologie, Institut für Festkörperphysik, Postfach 3640, D-76021 Karlsruhe

We have performed low-temperature scanning tunneling microscopy and spectroscopy on LiFeAs, Co doped NaFeAs and FeSe superconductors. The spectroscopy data routinely reveal important aspects of the electronic structure both very close to the Fermi level, i.e. the superconducting gap, and distinct features at higher energies. The latter appear in occupied states roughly between -0.3 eV and -0.5 eV in these materials, and allow specific comparison with ARPES band structure data.

TT 21.23 Mon 15:00 Poster B

Ferromagnetic Phase Transition in Li deficient LiFeAs — •Uwe Gräfe[1], Shiv Jee Singh[1], Robert Beck[1], Sabine Wurmehl[1,2], Christian Hess[1,3], and Bernd Büchner[1,2,3] — [1]IFW Dresden, Helmholtzstraße 20, 01069 Dresden — [2]TU Dresden Institut für Festkörperphysik, 01062 Dresden — [3]Center for Transport and Devices, Technische Universität Dresden, 01069 Dresden, Germany

While other iron pnictides only develop superconductivity under doping with holes or electrons, LiFeAs is a stoichiometric superconductor. So far doping, e.g. electron doping with Co [1] or Ni [2], is supressing the superconducting transition temperature. The same holds true for Li deficiency which formally corresponds to hole doping. This deficiency also leads to a ferromagnetic phase transition, evidenced by, e.g. magnetization and temperature dependent NQR measurements. Interestingly, upon doping LiFeAs with electrons, the NQR frequency at room temperature is shifted to lower values and vice versa for holes, i.e., the NQR frequency can be used as an absolute reference for the carrier doping in the material. Here we present systematic, NQR-controlled studies of the impact of various doping schemes on the structural, magnetic, and transport properties.

[1] Aswartham *et al.* 2011, PRB **84** 054534
[2] Pitcher *et al.* 2010, JACS **132** 10467

TT 21.24 Mon 15:00 Poster B

Superconductivity from Magnetic Fluctuations in $FeTe_{1-x}Se_x$-Feedback of Double Stripe Magnetism on Itinerant Spin Excitations — •Masoud Mardani[1], Johannes Knolle[2], Ilya Eremin[3], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany — [2]TCM Group, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom — [3]Institute for Theoretical

Physics III, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Iron-chalcogenide superconductors exhibit an unusual double stripe antiferromagnetic parent phase with ordering vector $Q_{AF} = (\pi/2,\pi/2)$ (in the one iron unit cell). In addition, magnetic excitations in optimally doped systems are peaked at momenta $Q_{SF} = (\pi,0)/(0,\pi)$, which is in contrast to most other families of iron-based superconductors. There, both the magnetic order of the parent compounds and the magnetic fluctuations in the superconducting state have the same momentum Q_{SF}, which is taken as a strong argument in favor of spin-fluctuation induced superconductivity. Here, we model iron-chalcogenides as a system of itinerant electrons coupled to localized electrons responsible for the double stripe magnetism. We study the feedback of this unusual magnetic order on the itinerant spin excitations at Q_{SF} and show that they increase with decreasing magnetism. We make connection to recent INS experiments and reproduce qualitatively the behavior of magnetic excitations in $FeTe_{1-x}Se_x$ from x=0 towards x=0.4.

TT 21.25 Mon 15:00 Poster B

Structural and superconducting properties of epitaxial $Fe_{1+y}Se_{1-x}Te_x$ thin films — •Stefan Richter[1], Feifei Yuan[1], Vadim Grinenko[1], Alberto Sala[2], Marina Putti[2], and Ruben Hühne[1] — [1]Institute for Metallic Materials IFW Dresden — [2]Dipartimento di Fisica, Università di Genova

The iron based superconductor Fe(Se,Te) is in the center of much ongoing research. The reason for this is on the one hand its simple crystal structure, that consists only of stacked Fe(Se,Te) layers so that structural and superconducting properties can be connected more easily, on the other hand FeSe itself shows a high sensibility for strain and changes in stoichiometry and can have potentially very high critical temperatures under hydrostatic pressure or in monolayers.

We investigate epitaxial thin films of $Fe_{1+y}Se_{1-x}Te_x$ grown by pulsed laser deposition on different single crystalline substrates. A high crystalline quality and a superconducting transition of up to about 20 K can be achieved using optimized deposition parameters. The influence of growth conditions, Te-doping, film thickness and post growth oxygen treatment on the structural and superconducting properties on these films will be presented in detail.

TT 21.26 Mon 15:00 Poster B

Coexistence of 3*d*-Ferromagnetism and Superconductivity in $(Li_{1-x}Fe_xOH)(Fe_{1-y}Li_ySe)$ — •Felix Brückner[1], Rajib Sarkar[1], Sirko Kamusella[1], Hubertus Luetkens[2], Ursula Pachmayr[3], Fabian Nitsche[3], Hans-Henning Klauss[1], and Dirk Johrendt[3] — [1]Institut für Festkörperphysik, Technische Universität Dresden, Germany — [2]Paul-Scherrer-Institut, Villigen, Switzerland — [3]Department Chemie, Ludwig-Maximilians-Universität München, Germany

In the family of iron-based superconductors, where the superconducting dome is usually separated from the magnetic phase, only few compounds show ferromagnetism arising in the superconducting state. The so far discovered examples show ferromagnetic ordering of Eu^{2+} ions. In this context, the presented ordering of iron orbitals in $(Li_{1-x}Fe_xOH)(Fe_{1-y}Li_ySe)$ is unique.

We performed a wealth of experimental methods to characterize the physics in this system, including dc resistivity and magnetization. With use of local probes (μSR,NMR,Mößbauer), we are able to describe the emergence of bulk ferromagnetism and superconductivity in a microscopic scale. Both phenomena can coexist, though they compete with each other, due to a spatial separation in the multilayer system.

TT 21.27 Mon 15:00 Poster B

Transport Properties of FeAs Single Crystals — •Matthias Gillig[1], Seunghyun Khim[1], Sabine Wurmehl[1,2], Bernd Büchner[1,2], and Christian Hess[1,3] — [1]Institute for Solid State Research, IFW Dresden, 01069 Dresden, Germany — [2]Technische Univeristät Dresden, 01069 Dresden, Germany — [3]Center for Transport and Devices, Technische Universität Dresden, 01069 Dresden, Germany

The electronic properties of all FeAs-based superconductors are primarily determined by the electronic states of the FeAs layers in these compounds. The physical properties of binary compound FeAs are therefore of general interest, despite the different structure as compared to that of hypothetical isolated FeAs-layers in the superconducting compounds. More specifically, FeAs crystallizes in an orthorhombic structure containing distorted $FeAs_6$ octahedra, instead of the $FeAs_4$ tetrahedra of the layers in the superconductors.

We have performed transport measurements on FeAs single crystals along all crystallographic directions. The resistivity is only weakly anisotropic and possesses a temperature dependence with a positive slope but a rather unusual non-linear behaviour. For temperatures $T \gtrsim 200$ K the resistivity is only weakly temperature dependent up to room temperature. However, below ~ 200 K the resistivity drops strongly upon cooling and exhibits a sharp kink at the spin density wave transition at ~ 70 K, resembling the unusual normal state resistivity of many Fe-based superconductors.

TT 21.28 Mon 15:00 Poster B

Superconducting properties and pseudogap from preformed Cooper pairs in the triclinic $(CaFe_{1-x}Pt_xAs)_{10}Pt_3As_8$ — •M. A. Surmach[1], F. Brückner[1], S. Kamusella[1], R. Sarkar[1], P. Y. Portnichenko[1], J. T. Park[2], G. Ghambashidze[3], H. Luetkens[4], P. Biswas[4], W. J. Choi[5], Y. I. Seo[5], Y. S. Kwon[5], H.-H. Klauss[1], and D. S. Inosov[1] — [1]TU Dresden, Germany — [2]MLZ, Garching, Germany — [3]MPI, Stuttgart, Germany — [4]PSI, Villigen, Switzerland — [5]DGIST, Daegu, Republic of Korea

Using μSR, INS and NMR, we investigated the novel Fe-based superconductor with a triclinic crystal structure $(CaFe_{1-x}Pt_xAs)_{10}Pt_3As_8$ ($T_c = 13$ K). The T-dependence of the superfluid density from the μSR measurements indicates the presence of two superconducting gaps. Our INS data revealed commensurate spin fluctuations at the $(\pi, 0)$ wave vector. Their intensity remains unchanged across T_c, indicating the absence of a spin resonance typical for many Fe-pnictides. Instead, we observed a peak around $\hbar\omega_0 = 7$ meV at the same wave vector, which persists above T_c and is characterized by the ratio $\hbar\omega_0/k_BT_c \approx 6.2$, i.e. significantly higher than typical values for the magnetic resonant modes in iron pnictides (~ 4.3). The T-dependence of magnetic intensity at 7 meV revealed an anomaly around $T^* = 45$ K related to the disappearance of this new mode. A suppression of the spin-lattice relaxation rate, $1 = /T_1T$, observed by NMR immediately below T^* without any notable subsequent anomaly at T_c, indicates that T^* could mark the onset of a pseudogap in $(CaFe_{1-x}Pt_xAs)_{10}Pt_3As_8$, likely associated with the emergence of preformed Cooper pairs.

TT 21.29 Mon 15:00 Poster B

$SrCo_2P_2$: a rare case of strong T dependence in the uncorrelated electronic DOS — •Christoph Bergmann, Helge Rosner, Yurii Prots, and Christoph Geibel — Max Planck Institut Chemical physics of solids, Dresden, Germany

Since the discovery of high temperature superconductivity in doped RFeAsO, transition metal pnictides have attracted considerable attention, especially those being close to a transition from a magnetic ordered to a non-magnetic ground state. $SrCo_2P_2$, a structural homologue of the AFe_2As_2 series of compounds, is such a system. Earlier investigation on polycrystals indicated a paramagnetic ground state, but a close proximity to magnetic ordering. Using a flux technique, we grew high quality single crystals with a residual resistivity ratio up to 150, and performed an in-depth study of the physical properties. Despite DFT calculation indicate a pronounced peak in the density of states at the Fermi level prone for electronic instability. We did not find any evidence for a phase transition. However we observed a quite unusual temperature dependence of the susceptibility with two distinct maxima, and Non-Fermi-liquid behavior in the resistivity at low temperature. Temperature dependent x-ray scattering experiments reveal an unusual behavior of the structural parameters, which induces a strong temperature dependence of the DOS at the Fermi edge. This provides a mechanism for the low temperature maximum, observed in the magnetic susceptibility.

TT 21.30 Mon 15:00 Poster B

QSGW+DMFT: an electronic structure scheme for the iron pnictides and beyond — •Jan Martin Tomczak — Institute of Solid State Physics, Vienna University of Technology, A-1040 Vienna, Austria

While in strongly correlated materials one often focuses on local electronic correlations, non-local exchange and correlation effects beyond band-theory can influence the physics of some systems even on a qualitative level. Here, I will argue that this is the case for the iron pnictide and chalcogenide superconductors. As an approach to tackle their electronic structure, I will detail the implementation of the recently proposed scheme that combines the quasi-particle self-consistent GW approach with dynamical mean-field theory: QSGW+DMFT [1,2]. I

will showcase the possibilities of QSGW+DMFT with a simplified application on $BaFe_2As_2$. Further, I will discuss the empirical finding that in the iron pnictides and chalcogenides dynamical and non-local correlation effects separate within the quasi-particle band-width.

[1] arXiv:1411.5180.
[2] Phys. Rev. Lett. 109, 237010 (2012).

TT 21.31 Mon 15:00 Poster B

Persistent circular currents around holes in graphite interfaces — •Bogdan Semenenko, Annette Setzer, Winfried Böhlmann, and Pablo Esquinazi — Division of Superconductivity and Magnetism, Institut für Experimentelle Physik II, Universität Leipzig, D-04103 Leipzig, Germany

To prove the existence of persistent circular currents around artificially made holes in graphite flakes with embedded interfaces we used highly oriented pyrolytic graphite (HOPG) with a large density of interfaces. The presence of interfaces in HOPG is responsible for the metallic-like behavior as well as for the superconductivity found in some graphite materials [1,2]. We performed high precision magnetic measurements using a SQUID at temperatures from 5 K to 300 K and maximum magnetic fields between 0.05 T and 5 T applied normal to the holes area. The holes of ~ 2 μm diameter were produced using a focused Ga^+ beam microscope. The rest of the graphite surface was protected by a thick layer of PMMA. The measurements show that if we drill holes in the HOPG it is possible to see a relatively large magnetic moment, which remains persistent after removing the applied field. We speculate that this signal originates from circular currents around the holes that flow at the different interfaces (about 100 within the thickness of the graphite flake used).

[1] P. Esquinazi, T. T. Heikkilä, Y. V. Lysogoskiy, D. A. Tayurskii, and G. E. Volovik, JETP Letters **100**, 336 (2014).
[2] A. Ballestar et al., New Journal of Physics **15**, 023024 (2013).

TT 21.32 Mon 15:00 Poster B

Andreev reflections in single C_{60} junctions — •Jonathan Brand, Nicolas Néel, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

Single C_{60} molecules deposited on an ultrathin oxide film on Nb(110) were investigated using a low-temperature scanning tunnelling microscope. Spectroscopy of the differential conductance (dI/dV) in the tunnelling range reveals proximity-induced superconductivity in junctions comprising the oxide layer as well as single C_{60} molecules. Andreev reflections are enhanced upon controllable fabrication of tip-surface contacts, which is reflected by the gradual transformation of the superconducting energy gap into a characteristic zero-bias peak in dI/dV spectra. The current-voltage characteristics of the tunnelling and contact junctions are modelled within the Blonder-Tinkham-Klapwijk theory [1].

[1] G. E. Blonder, M. Tinkham, and T. M. Klapwijk, Phys. Rev. B **25**, 4515 (1982).

TT 21.33 Mon 15:00 Poster B

Ordinary and Triplet Superconducting Spin Valve Effect in Fe/Pb based systems — •Pavel Leksin[1], Nadir Garifyanov[2], Ilgiz Garifullin[2], Yakov Fominov[3], Joachim Schumann[1], Yulia Krupskaya[1], Vladislav Kataev[1], Christian Hess[1], Oliver Schmidt[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, Germany — [2]Zavoisky Physical-Technical Institute of RAS, Kazan, Russia — [3]L. D. Landau Institute for Theoretical Physics of RAS, Moscow, Russia

We report on experimental evidence for the occurrence of the long range triplet correlations (LRTC) of the superconducting (SC) condensate in the spin-valve heterostructures CoO_x/Fe1/Cu/Fe2/Pb [1]. The LRTC generation in this layer sequence is accompanied by a T_c suppression near the orthogonal mutual orientation of the Fe1 and Fe2 layers' magnetization. This T_c drop reaches its maximum of 60mK at the Fe2 layer thickness $d_{Fe2} = 0.6$ nm and falls down when d_{Fe2} is increased. The modification of the Fe/Pb interface by using a thin Cu layer between Fe and Pb layers reduces the SC transition width without preventing the interaction between Pb and Fe2 layers. The dependence of the SSVE magnitude on Fe1 layer thickness d_{Fe1} reveals maximum of the effect when d_{Fe1} and d_{Fe2} are equal and the d_{Fe2} value is minimal [2]. Using the optimal d_{Fe1}, d_{Fe2} and the intermediate Cu layer we realized almost full switching from normal to SC state due to SSVE.

[1] P. V. Leksin et al, Phys. Rev. Lett. 109, 057005 (2012).
[2] P. V. Leksin et al., JETP Lett., vol. 97, iss. 8 (2013).

TT 21.34 Mon 15:00 Poster B

Thickness Dependence of the Triplet Spin-Valve Effect in Superconductor-Ferromagnet Heterostructures — •Daniel Lenk[1], Vladimir I. Zdravkov[1,2], Jan Kehrle[1], Günther Obermeier[1], Roman Morari[1,3], Hans-Albrecht Krug von Nidda[1], Claus Müller[1], Anatolie S. Sidorenko[3], Siegfried Horn[1], Reinhard Tidecks[1], and Lenar Tagirov[4] — [1]Institut für Physik, Universität Augsburg, D-86159 Augsburg, Germany — [2]Present address: Institut für angewandte Physik, Universität Hamburg, D-20355 Hamburg, Germany — [3]D. Ghitsu Institute of Electronic Engineering and Nanotechnologies ASM, MD 2028 Kishinev, Moldova — [4]Solid State Physics Department, Kazan Federal University, 420008 Kazan, Russia

We investigated the triplet spin-valve effect in nanoscale layered $S/F_1/N/F_2/AF$ heterostructures with varying F_1-layer thickness (where S=Nb is a singlet superconducting, F_1=$Cu_{41}Ni_{59}$ and F_2=Co a ferromagnetic, and N a normal-conducting, non-magnetic layer). The theory predicts a long-range, odd-in-frequency triplet component of superconductivity at non-collinear alignment of the magnetizations of F_1 and F_2. This triplet component exhausts the singlet state and, thus, lowers the superconducting transition temperature, T_c, yielding a global minimum of T_c close to the perpendicular mutual orientations of the magnetizations. We found an oscillating decay of T_c suppression, due to the generation of the triplet component, with increasing F_1 layer thickness, which we discuss in the framework of recent theories. This work was supported by DFG Grant No. HO955/9-1.

TT 21.35 Mon 15:00 Poster B

Josephson Currents in a Weak-Link Superconductor-Ferromagnet Proximity Structure — •Jan Gelhausen[1] and Matthias Eschrig[2] — [1]Royal Holloway, University of London, United Kingdom, Universität zu Köln — [2]Royal Holloway, University of London, United Kingdom

We provide theoretical support for experimental measurements on a weak-link hybrid structure consisting of superconducting elements that are influenced by a ferromagnet (SSFS). It consists of a thin Aluminium wire that runs across a ferromagnetic disc made out of Nickel. The experimentally measured phase diagram allows for an identification of several temperature dependent system states. We numerically calculate important physical observables such as the local density of states, singlet and triplet pair amplitudes, proximity induced minigaps and their scaling behaviour with the system size, spin-magnetisations and the phase and temperature dependence of Josephson currents. The current-phase relationship of the SSFS junction is multivalued for low temperatures and approaches a sinusoidal form for increasing temperatures. This behaviour is indicative of a crossover from a Josephson-like behaviour to a junction that is dominated by a depairing current for decreasing temperatures.

TT 21.36 Mon 15:00 Poster B

Nonlocal spin-transport measurement of superconductor-ferromagnet nanostructures — •Stefan Kolenda, Michael J. Wolf, Florian Hübler, and Detlef Beckmann — Institut für Nanotechnologie, Karlsruher Institut für Technologie

We present measurements of the nonlocal conductance of nanostructures with several ferromagnetic electrodes lying perpendicular on a superconducting wire. In these strucures nonlocal conductance is mostly given by diffusion of quasiparticles, which are injected by one of the electrodes and detected by an other one. Applying a magnetic field induces a Zeeman splitting in the quasiparticals density of states, which suppreses the relaxation of injected spin imbalance, thus spin transport over distances of several micrometers is found [1][2]. While in the previous experiments the magnetic field was aligned parallel to the ferromagnetic electrodes, we also show measurements applying the magnetic field noncollinear with the magnetization of the ferromagnetic electrodes. We compare our results to the previous case.

[1] F. Hübler *et al.*, Phys. Rev. Lett. **109**, 207001 (2012)
[2] C.H.L. Quay *et al.*, Nature Phys. **9**, 84 (2013)

TT 21.37 Mon 15:00 Poster B

Upper Critical Field and Vortices in S/F Bilayers Exhibiting the Quasi-Onedimensional FFLO-like State — Daniel Lenk[1], •Mamoun Hemmida[1], Jan Kehrle[1], Vladimir I. Zdravkov[1,2], Aladin Ullrich[1], Günther Obermeier[1], Roman Morari[1,3],

Claus Müller[1], Anatolie S. Sidorenko[3], Alois Loidl[1], Hans-Albrecht Krug von Nidda[1], Lenar Tagirov[1,4], Siegfried Horn[1], and Reinhard Tidecks[1] — [1]Institut für Physik, Universität Augsburg, D-86159 Augsburg, Germany — [2]Present address: Institut für angewandte Physik, Universität Hamburg, D-20355 Hamburg, Germany — [3]D. Ghitsu Institute of Electronic Engineering and Nanotechnologies ASM, MD 2028 Kishinev, Moldova — [4]Solid State Physics Department, Kazan Federal University, 420008 Kazan, Russia

We investigate the temperature dependence of the upper critical field, B_{c2}, in superconductor/ferromagnet (S/F) bilayers as a function of the F-layer thickness, d_F, by resistance measurements. We extracted GL coherence lengths and estimated an effective thickness of the superconducting layer by evaluating the perpendicular coherence length at the 3D-2D crossover temperature in the parallel B_{c2}. We found an unexpected non-monotonous behavior of the effective thickness as a function of d_F. Moreover, we investigated the anisotropy of B_{c2} by microwave absorption. The results show a deviation from Tinkham's prediction for thin films, which we attribute to the additional anisotropy induced by the quasi-1D FFLO-like state. Thus, we propose a new type of vortex, developing in the S/F bilayer in magnetic fields applied close to parallel. This work was supported by DFG Grant No. HO955/9-1.

TT 21.38 Mon 15:00 Poster B

Non-equilibrium spin and charge transport in superconducting heterojunctions — •Marcel Thalmann, Marcel Rudolf, Julian Braun, Torsten Pietsch, and Elke Scheer — Department of Physics, University of Konstanz, Universitätsstraße 10, 78464 Konstanz, Germany

Ferromagnet Superconductance (F/S) junctions are rich in exciting quantum-physical-phenomena, which are still poorly understood but may provide bright prospects for new applications. In contrast to conventional normal-metal proximity systems, Andreev reflection is suppressed for singlet cooper pairs in F/S heterostructures. However, long-range triplet pairing may be observed in S/F systems with non-collinear magnetization or spin-active interfaces.

Herein, we investigate non-equilibrium transport properties of lateral S/F heterojunctions, defined via electron beam lithography. In particular we focus microwave- and magneto-transport spectroscopy on conventional type-I (Al, Pb, Zn) and type-II (Nb) superconductors in combination with strong transition metal ferromagnets (Ni, Co, Fe). A cryogenic HF readout platform and advanced electronic filtering is developed and results on Al-based heterojunctions are shown.

TT 21.39 Mon 15:00 Poster B

Measurement setup for the magnetic penetration depth and superfluid stiffness in thin superconducting films. — •Lorenz Fuchs[1], Markus-Christopher-Paul Brunner[1], Jessica Bousquet[2], Ina Schneider[1], Klaus Kronfeldner[1], Etienne Bustarret[2], and Christoph Strunk[1] — [1]Institute for exp. and appl. Physics, University of Regensburg, Germany — [2]Institut NÉEL, Grenoble, France

A mutual inductance measurement setup has been established in order to determine the magnetic penetration depths of thin film superconductors. [1] By measuring the variation of the mutual inductance M, the temperature dependent penetration depth can be evaluated. [2] The setup has been characterized using thin aluminum and niobium films as a reference. Temperature dependence of λ of B-doped diamond films is determined down to 0.3K and compared with theoretical expectations. [3] The impact of the doping ratio B/C and film thickness on λ and T_c is investigated. Correlation between the film impedance $\sigma = \sigma_1 - i\sigma_2$ and λ is examined.

[1] A.T. Fiory et al., Appl. Phys. Lett. **52** (25), 1988
[2] T. Lemberger et al., J. Appl. Phys. **83** (8), 1998
[3] E. Bustarret et al., Phil. Trans. R. Soc. A, 2008

TT 21.40 Mon 15:00 Poster B

Simulation of electronic structure Hamiltonians in a superconducting quantum computer architecture — •Michael Kaicher[1], Peter J. Love[2], and Frank K. Wilhelm[1] — [1]Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Department of Physics, Haverford College, Haverford, Pennsylvania 19041, USA

Quantum chemistry has become one of the most promising applications within the field of quantum computation. Simulating the electronic structure Hamiltonian (ESH) in the Bravyi-Kitaev (BK)-Basis to compute the ground state energies of atoms/molecules reduces the number of qubit operations needed to simulate a single fermionic operation to O(log(n)) as compared to O(n) in the Jordan-Wigner-Transformation. In this work we will present the details of the BK-Transformation, show an example of implementation in a superconducting quantum computer architecture and compare it to the most recent quantum chemistry algorithms suggesting a constant overhead.

TT 21.41 Mon 15:00 Poster B

Giant Atom Coupled to Surface Acoustic Waves — •Lingzhen Guo, Anton Kockum, and Göran Johansson — Department of Microtechnology and Nanoscience, MC2, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden

We investigate the system of an artificial atom (transmon) coupled to surface acoustic waves (SAWs). The artificial atom is giant because the wavelength of SAWs is much smaller than that of light and comparable to the length scale of transmon. We study the situation that the giant atom has two "legs" coupling to SAWs confined in a 1D transmission line. We investigate the parameter regime where the travelling time T of SAWs between the two legs is arbitrary long. We use the time delay differential equations to describe our system and find some new phenomena when the travelling time T is much longer than the atom's relaxation time, e.g., the decay of the whole system follows a type of polynomial decay instead of exponential decay. We also investigate the transmission properties under driving and find more interesting properties of this system beyond the Markov approximation. The results we get are also true for similar systems implemented in the light cavities and circuit QED.

TT 21.42 Mon 15:00 Poster B

Terahertz emission and electromagnetic waves in single crystal $Bi_2Sr_2CaCu_2O_8$ structures — •Raphael Wieland[1], Fabian Rudau[1], Boris Gross[1], Nickolay Kinev[2], Manabu Tsujimoto[3], Min Ji[4,5], Ya Huang[4,5], Xianjing Zhou[4,5], Deyue An[4,5], Thomas Judd[1], Peihang Wu[5], Takeshi Hatano[4], Huabing Wang[4,5], Valery Koshelets[2], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Physikalisches Institut and Center for Collective Quantum Phenomena in LISA$^+$, Universität Tübingen, Tübingen, Germany — [2]Kotel'nikov Institute of Radio Engineering and Electronics, Moscow, Russia — [3]Kyoto University, Kyoto, Japan — [4]National Institute for Materials Science, Tsukuba, Japan — [5]Research Institute of Superconductor Electronics, Nanjing University, Nanjing, China

Josephson Junctions (JJs) offer a natural way to convert a dc voltage into high-frequency electromagnetic radiation. In the high-Tc superconductor $Bi_2Sr_2CaCu_2O_8$ (BSCCO), JJs form intrinsically, allowing to fabricate stacks of hundreds of junctions easily. Emission can occur at relatively low bias currents but also at larger input power with frequencies from 0.4 to 1 THz. At high bias, a hot spot forms, affecting both the intensity and the linewidth of the radiation. BSCCO mesas are believed to work as a cavity for electromagnetic standing waves, synchronizing all the junctions in the stack. We investigated THz emission and hotspot formation using a combination of transport measurements, electromagnetic wave detection via a superconducting receiver and low temperature scanning laser microscopy.

TT 21.43 Mon 15:00 Poster B

Sensitive YBCO nanoSQUIDs for the investigation of small spin systems — •Benedikt Müller[1], Tobias Schwarz[1], Roman Wölbing[1], María José Martínez-Pérez[1], Christopher F. Reiche[2], Thomas Mühl[2], Bernd Büchner[2], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut and Center for Collective Quantum Phenomena in LISA$^+$, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [2]Leibniz Institute for Solid State and Materials Research IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany

We report on advances in the realization of dc YBCO nanoSQUIDs for continuous measurement of magnetic nanoparticle magnetization loops in strong magnetic fields up to the Tesla range, applied in the plane of the SQUID loop at temperatures of 4 K and below. Our grain boundary junction based YBCO SQUIDs are patterned by focused ion beam milling and feature a constriction next to the SQUID loop, allowing for on-chip SQUID modulation and bias reversal readout schemes.

Using numerical simulations based on London theory, the spin sensitivity $S_\mu^{1/2} = S_\Phi^{1/2}/\phi_\mu$ was improved by optimizing both the flux noise $S_\Phi^{1/2}$ and the coupling factor $\phi_\mu = \Phi/\mu$ (Φ is the magnetic flux coupled into the SQUID loop by a particle with magnetic moment μ). For opti-

mized experimental devices, flux noise levels down to $50\,\mathrm{n}\Phi_0/\mathrm{Hz}^{1/2}$ in the white noise limit have been achieved, corresponding to a calculated spin sensitivity of only a few $\mu_\mathrm{B}/\mathrm{Hz}^{1/2}$.

Further, the magnetization reversal of a Fe filled carbon nanotube attached to a YBCO nanoSQUID was traced out.

TT 21.44 Mon 15:00 Poster B

Characterization of Josephson parametric amplifiers — •Stefan Pogorzalek[1,2,3], Kirill Fedorov[1,2,3], Ling Zhong[1,2,3], Martin Bitzenbichler[1,2,3], Max Haeberlein[1,2,3], Manuel J. Schwarz[1,2,3], Peter Eder[1,2,3], Jan Goetz[1,2,3], Friedrich Wulschner[1,2,3], Edwar Xie[1,2,3], Alexander Baust[1,2,3], Achim Marx[1,2,3], Edwin P. Menzel[1,2,3], Frank Deppe[1,2,3], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

Propagating quantum microwaves are a promising building block for quantum communication. In particular, such itinerant quantum microwaves can be generated in the form of squeezed photon states using Josephson parametric amplifiers (JPA). A thorough experimental characterization of JPAs is therefore an essential prerequisite for further experiments towards quantum communication. For implementing JPAs we employ an established $\lambda/4$ bi-coplanar microwave resonator design where a dc-SQUID is biased by an external flux to tune the resonant frequency. An inductively coupled antenna acts as a pump for the JPA. We characterize several JPAs and evaluate the data within standard Josephson junction theory and the input-output formalism. In particular, we investigate hysteretic and bifurcation behavior of the JPAs in addition to usual non-degenerate JPA gain measurements.

This work is supported by the DFG via SFB 631 and the EU projects CCQED and PROMISCE.

TT 21.45 Mon 15:00 Poster B

Temperature dependence of coherence in transmon qubits — •Steffen Schlör[1], Jochen Braumüller[1], Oleksandr Lukashenko[1], Hannes Rotzinger[1], Martin Sandberg[2], Michael R. Vissers[2], David P. Pappas[2], Martin Weides[1], and Alexey V. Ustinov[1] — [1]Physikalisches Institut, KIT, 76131 Karlsruhe, Germany — [2]NIST, Boulder, CO 80305, United States

Superconducting qubits are a promising field of research, not only with respect to quantum computing but also as highly sensitive detectors and due to the possibility of using them to study fundamental implications of quantum mechanics. The requirements for qubits that can be used as building blocks in a potential quantum computer are challenging. Modern superconducting qubits like the transmon are strong candidates for achieving these goals. The main challenge here is to increase the coherence of prepared quantum states. Here, we experimentally investigate the influence of temperature variation on relaxation and dephasing of a transmon qubit. Our goal is to understand decoherence mechanisms in material optimized circuits. Aiming at longer coherence, in this case peaking over $50\,\mu\mathrm{s}$ for T_1 and T_2, our samples are fabricated at NIST using two different materials. Low-loss TiN was used for the shunt capacitance as well as the resonator, combined with shadow evaporated ultra-small Al-$\mathrm{AlO_x}$-Al Josephson junctions. We will present temperature-dependent data on qubit relaxation and dephasing times as well as power spectra. Our data will be compared to previously obtained temperature dependent data for other types of qubits.

TT 21.46 Mon 15:00 Poster B

Collective coupling of tunable transmon array via a cavity bus — •Ping Yang, Martin Weides, and Alexey V. Ustinov — Physikalisches Institut, KIT, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Germany

Nowadays, superconducting multi-qubit circuits can be fabricated and studied experimentally. In order to manipulate the propagation of electromagnetic waves and explore the scalability of superconducting qubit circuits, we investigate coplanar waveguide resonators coupled to up to eight transmon qubits. An array of transmons can be viewed as a quantum metamaterial. Compared to a metamaterial made of flux qubits [1], our current approach using transmons anticipates smaller parameter spread and is easier to fabricate. The resonators are fabricated using optical lithography, while the qubits are made by using electron-beam lithography. Every qubit is biased individually via a flux-bias line. Thus, the interaction between the individual qubit and the resonator can be easily turned on and off by tuning the qubit eigenfrequencies. The simultaneous readout is implemented by measuring the dispersive shift of the resonator. This scheme enables one to study the collective behavior (Dicke state, quantum synchronization, superradiance) between all, or a subset of qubits.

[1] P. Macha, et al. Nature Commun. 5, 5146 (2014)

TT 21.47 Mon 15:00 Poster B

Quantum Phase-Slips in Superconducting AlO_x Nanowire Arrays at Microwave Frequencies — •Sebastian T. Skacel[1], Marco Pfirrmann[1], Jan N. Voss[1], Julian Münzberg[1], Lucas Radtke[1], Sebastian Probst[1], Martin Weides[1,2], Hannes Rotzinger[1], Hans E. Mooij[1,3], and Alexey V. Ustinov[1,4] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, D-55128 Mainz, Germany — [3]Kavli Institute of Nanoscience, Delft University of Technology, 2628 CJ Delft, The Netherlands — [4]Russian Quantum Center, 100 Novaya St., Skolkovo, Moscow region, 143025, Russia

Superconducting nanowires in the quantum phase slip (QPS) regime allow to study the flux and phase dynamics in duality to Josephson junction systems. However, due to the vanishing self-capacitance of the nanowires, the microwave response significantly differs. We experimentally study parallel arrays of nanowires which are embedded in a resonant circuit at GHz frequencies. The samples are probed at ultra-low microwave power and applied magnetic field at mK temperatures. The AlO_x nanowires, with a sheet resistance in the kΩ range, are fabricated by sputter deposition of aluminium in a controlled oxygen atmosphere. The wires are defined with conventional electron beam lithography down to a width of approximately 15 nm. We present the fabrication of the nanowire arrays and measurement results for arrays coupled to superconducting microwave resonators.

TT 21.48 Mon 15:00 Poster B

How to identify quantum effects in a driven current-biased JJ — •Harald Losert, Karl Vogel, and Wolfgang P. Schleich — Institut für Quantenphysik, Universität Ulm, D-89069 Ulm, Germany

The phase difference in a current-biased Josephson junction behaves like a particle in a tilted washboard potential. There has been a huge interest in the behaviour of such a particle - in particular in the case of an external periodic driving field - since the escape of the phase-particle corresponds to the voltage switching of the associated Josephson junction. Experimentally, the bias current is increased until the voltage state changes. Quantum mechanically it can be explained as tunneling from the ground state, or from an excited state. However, the resulting switching current distribution can also be explained classically [1]. Up to now, the distinction between quantum and classical effects is still an open question in many implementations of Josephson junctions.

Based on this discussion, we present numerical simulations of the quantum mechanical and classical time evolution of such a system. In particular, we contrast the resulting switching current distributions.

[1] Grønbech-Jensen *et al.*, *Phys. Rev. Lett.* **95**, 067001 (2005).

TT 21.49 Mon 15:00 Poster B

SQUIDs for the readout of metallic magnetic calorimeters — •Anna Ferring, Mathias Wegner, Andreas Fleischmann, Loredana Gastaldo, Sebastian Kempf, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Germany.

Superconducting quantum interference devices (SQUIDs) are the devices of choice to read out metallic magnetic calorimeters (MMCs). Here, the temperature change of the detector upon the absorption of an energetic particle is measured as a magnetization change of a paramagnetic temperature sensor that is situated in a weak magnetic field. Driven by the need for devices that allow for the readout of large-scale detector arrays with hundreds or even thousands of individual detectors as well as of single channel detectors with sub-eV energy resolution, we have recently started the development of low-T_c current-sensing SQUIDs. In particular, we are developing cryogenic frequency-domain multiplexers based on non-hysteretic rf-SQUIDs for detector array readout as well as dc-SQUIDs for single channel detector readout. We discuss our SQUID designs and the performance of prototype SQUIDs. We particularly focus on the frequency and temperature dependence of the SQUID noise as well as the reliability of our SQUID fabrication process for Nb/Al-AlO_x/Nb Josephson junctions. Additionally, we demonstrate experimentally that state-of-the-art MMCs can successfully be read out with our current devices. Finally, we discuss different strategies to improve the SQUID and de-

tector performance aiming to reach sub-eV energy resolution for individual detectors as well as for detector arrays.

TT 21.50 Mon 15:00 Poster B

Metallic Magnetic Calorimeters for high resolution X-ray spectroscopy — •M. Krantz, D. Hengstler, J. Geist, C. Schötz, K. Hassel, S. Hendricks, M. Keller, S. Kempf, L. Gastaldo, A. Fleischmann, and C. Enss — KIP Heidelberg University.

We develop microfabricated, energy dispersive particle detector arrays based on metallic magnetic calorimeters (MMCs) for high resolution x-ray spectroscopy to challenge bound-state QED calculations. Our MMCs are operated at about T=30 mK and use a paramagnetic temperature sensor, read-out by a SQUID, to measure the energy deposited by single x-ray photons. We discuss the physics of MMCs, the detector performance and the cryogenic setups for two different detector arrays. We present their microfabrication layouts with focus on challenges like the heatsinking of each pixel of the detector and the overhanging absorbers. The maXs-20 detector is a linear 1x8-pixel array with excellent linearity in its designated energy range up to 20 keV and unsurpassed energy resolution of 1.6 eV for 6 keV x-rays. MaXs-20 operated in a highly portable pulse tube cooled ADR setup has already been used at the EBIT facilities of the MPI-K for new reference measurements of V-like and Ti-like tungsten. The maXs-30 detector currently in development is a 8x8-pixel 2d-array with an active detection area of 16 mm^2 and is designed to detect x-rays up to 50 keV with a designated energy resolution below 5 eV. MaXs-30 will be operated in a cryogen free 3He/4He-dilution refrigerator at the tip of a 40 cm long cold finger at $T = 20$ mK.

TT 21.51 Mon 15:00 Poster B

A large-area 4k-pixel detector for position and energy resolving detection of neutral molecular fragments — •D. Schulz[1], L. Gamer[1], A. Fleischmann[1], L. Gastaldo[1], S. Kempf[1], C. Krantz[2], O. Novotny[3], A. Wolf[2], and C. Enss[1] — [1]KIP Heidelberg University. — [2]MPI-K Heidelberg. — [3]Columbia Astrophysics Laboratory, New York, USA.

To investigate reactions like dissociative recombination in a laboratory environment, the Max Planck Institute for Nuclear Physics in Heidelberg is commissioning the Cryogenic Storage Ring to prepare molecular ions in their rotational and vibrational ground state. The full kinematics of these processes can be resolved by a position and energy sensitive detection of the produced neutral molecular fragments.

We present the design of a new large-area multi-pixel detector using metallic magnetic calorimeters for position and energy sensitive detection of massive particles with kinetic energies of up to a few hundred keV. The detector encompasses an array of 4096 quadratic absorbers, each with a side length of 700 μm, amounting to a total detection area of about 20 cm^2. Groups of four absorbers are thermally connected to one paramagnetic sensor, using different thermal links for pixel discrimination. A temperature change in the paramagnetic sensor leads to a change of magnetization in the sensor. Thanks to a novel readout scheme, all 4096 sensors can be read out using at total of 32 SQUIDs only.

TT 21.52 Mon 15:00 Poster B

Thermodynamical properties of Au:Ho dilute alloys for the ECHo collaboration — •Sebastian Haehnle — for the ECHo collaboration (http://www.kip.uni-heidelberg.de/echo/members), KIP Heidelberg University.

The absolute scale of the neutrino mass eigenstates is one of the puzzles in modern particle physics. One method to investigate the value of the electron neutrino mass is to analyse the high energy region of the ^{163}Ho electron capture spectrum. In the ECHo experiment low temperature metallic magnetic calorimeters are used for the calorimetric measurement of the EC spectrum of ^{163}Ho. To ensure 100% quantum efficiency the ^{163}Ho ions are implanted into the gold absorber. A detailed study of the thermodynamical properties of highly diluted Au:Ho is necessary to determine the detector response and to define the highest concentration possible for which the performance of the detectors is not reduced.

We determined Crystal-Field parameters for holmium in gold based on magnetization measurements from 2 K to 300 K, that would result in a non-Kramers doublet as groundstate with the first excited triplet state at 140 mK. We used numerical calculations for the combined Hamiltonian of the Crystal-Field and the Hyperfine interaction to predict a theoretical heat capacity at millikelvin temperatures. The results of the numerical calculation are compared to experimental results.

TT 21.53 Mon 15:00 Poster B

Microfabricated Thick Proximity Bi-layers as Sensors for Magnetic Penetration Thermometers (MPTs) — •J. Geist, D. Hengstler, M. Keller, M. Krantz, C. Schötz, S. Kempf, L. Gastaldo, A. Fleischmann, and C. Enss — Kirchhoff-Institute for Physics - Heidelberg University

Metallic magnetic calorimeters for high resolution x-ray spectroscopy use dilute paramagnetic alloys as temperature sensors operated at a temperature of 20 mK. Recent prototypes for soft x-rays achieved an energy resolution of 1.6 eV(FWHM) for 6 keV photons. To reach a similar resolution at higher and easy accessible temperatures, we are presently investigating superconducting sensor materials. Thereby the steep temperature dependence of the magnetic penetration depth is used in the superconducting transition as temperature information. A technically interesting class of materials might be proximity bi-layers consisting of a thick normal metal layer and a superconductor. This combination might allow to tune not only T_c, but also the transition width and therefore the dynamic range. We present first results of measurements were a thick gold and silver layer is deposited onto aluminum. The bi-layers are patterned to form meander-shaped coils, where the temperature dependence of the coil inductance was studied in inductance bridge circuits with SQUID readout. We present data for different structure sizes and discuss the resulting expected signal height and energy resolution.

TT 21.54 Mon 15:00 Poster B

Development of RF-SETs for error detection in semiconductor electron pumps — •David Reifert, Niels Ubbelohde, Ralf Dolata, Lukas Fricke, Thomas Weimann, and Alexander Zorin — Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig. Germany

Semiconductor single electron pumps allow the transport of single electrons with a frequency f (about 1 GHz) which results in a current (I=e*f) in the range of about 0.1 nA. However, since the accuracy of these pumps (at present still worse than 1 ppm) is not sufficient for metrological applications, we developed a method to detect and account the errors of these pumps, which should lead to an improved accuracy. To realise this error detection we put several electron pumps in a serial circuit with intermediate charge islands between them. If one of the pumps operating simultaneously makes an error the charge on the island changes stepwise which can be detected by a sensitive charge detector. We use superconducting Al single electron transistors (SETs) as ultra-sensitive charge detectors which are capacitively coupled to the intermediate charge islands. In our previous experiments we operated the SETs in DC mode which allowed rather slow measurement bandwidth of a few kHz. To increase the measurement bandwidth of the SETs we put them in a resonant tank circuits and measure the reflectance of these resonators at corresponding frequencies. This tank circuit matches the high impedance of the SET (>100 kOhm) to a 50 Ohm line. We will show the general measurement setup and some first measurements of charge detection with such a RF-SET.

TT 22: Other Low Temperature Topics: Poster Session

Time: Monday 15:00–18:00 Location: Poster B

TT 22.1 Mon 15:00 Poster B

Quantum Monte Carlo Results for the Breathing Mode of Trapped Bosons — •Tobias Dornheim, Alexei Filinov, and Michael Bonitz — Institut für Theoretische Physik und Astrophysik der Christian-Albrechts-Universität zu Kiel, Leibnizstraße 15, 24098 Kiel, Germany

The quantum breathing mode (QBM, e.g. [1]) is of fundamental interest for the investigation of harmonically confined systems since it might serve as a tool of diagnostics [2]. We perform ab initio path integral Monte Carlo (PIMC) [3] simulations for up to N=1000 particles in TD equilibrium and investigate the QBM for both dipole- and Coulomb-interacting bosons using a recently developed improved sum-rule formalism [4]. We study the dependence on the particle number N and coupling strength λ for 2D and 3D systems and observe a transition towards the classical limit with increasing system size and interaction.

[1] J. W. Abraham and M. Bonitz, Contrib. Plasma Phys. **54**, 27-99 (2014)
[2] C. R. McDonald et al., Phys. Rev. Lett. **111**, 256801 (2013)
[3] M. Boninsegni et al., Phys. Rev. E **74**, 036701 (2006)
[4] J. W. Abraham et al., New J. Phys. **16**, 013001 (2014)

TT 22.2 Mon 15:00 Poster B

Metallic Coplanar Microwave Resonators for Cryogenic Applications — •Mojtaba Javaheri[1], Conrad Clauss[1], Daniel Bothner[2], Dieter Koelle[2], Reinhold Kleiner[2], Martin Dressel[1], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — [2]Physikalisches Institut and Center for Collective Quantum Phenomena in LISA$^+$, Universität Tübingen, Tübingen, Germany

Microwave (MW) spectroscopy based on resonator measurements can reveal important information about charge and spin dynamics in solids. Recently superconducting coplanar resonators, which are commonly used in quantum information science, have successfully been compatibilized and applied for cryogenic magnetic resonance studies. However, they feature certain disadvantages arising from the magnetic-field dependence of the superconductivity and also diamagnetic field repulsions. To avoid this, we now study metallic (non-superconducting) coplanar resonators as an alternative approach for applications at cryogenic temperatures and finite magnetic fields.

We have prepared coplanar MW resonators made of either copper or gold (thin) films with various geometrical specifications. Their MW performance in the frequency range of 1 GHz to 18 GHz and at temperatures between 5 K and 300 K are measured. We find the temperature dependence of the resonator quality factor corresponds to the dc conductivity. We present some strategies to optimize the MW properties of the metallic films and the actual resonator device. The results are compared to some previous studies on superconducting resonators.

TT 22.3 Mon 15:00 Poster B

Compact 11 mK scanning tunneling microscope — •Timofey Balashov and Wulf Wulfhekel — Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany

A new scanning tunneling microscope (STM) working at 11 mK with low noise, high stability and high energy resolution was developed for the measurement of magnetic and vibronic excitations.

Advances in dilution refrigerator technology allow for a compact design with direct transfer under vision of both tip and sample into the STM, as well as material deposition at low temperature. An additional vacuum chamber serves for in-situ preparation of tips and samples.

The cryostat reaches the operating temperature in less than 5 hours after sample transfer, and has a low helium consumption of less than 200 ml/hour. A superconducting coil provides an out-of-plane magnetic field of up to 8 Tesla (projected). The vertical stability of the tunnel junction is below 1 pm (peak to peak) and the electric noise floor of tunneling current is about $2\,\mathrm{fm}/\sqrt{\mathrm{Hz}}$.

TT 22.4 Mon 15:00 Poster B

Pulse Tube Cryocoolers at 4 K: Optimized Design for Low Vibrations and Temperature Oscillations — •Jens Falter[1], Bernd Schmidt[1,2], Andreas Euler[1], Marc Dietrich[1,2], André Schirmeisen[1,2], and Günter Thummes[1,2] — [1]TransMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany — [2]Institute of Applied Physics (IAP), Justus-Liebig-University Giessen, Germany

Since their invention [1] two-stage 4 K pulse tube cryocoolers (PTCs) have evolved as an excellent technique for "dry" cooling of cryogenic experiments without need for liquid helium, operating even below 4 K. PTCs have no cold moving mechanical parts, which is a main advantage over conventional Gifford-McMahon coolers. This results in a lower vibration level and long operation times. These properties make PTCs very attractive as the main cooling system for applications with high demands for low vibrations and high temperature stability. However, PTCs still exhibit two intrinsic effects due to the cyclic compression and expansion of the working fluid (He) in the cold head: (a) a periodic elastic deformation ("breathing") of the thin walled pulse- and regenerator-tubes, which leads to residual vibrations and (b) a periodic variation in temperature. Here, we present optimized applications of two-stage 4 K PTC cold heads to reduce these effects. First, both intrinsic effects are minimized by adapting the input power of the compressor. Remaining vibrations are reduced by mechanical decoupling of the experiment from the cold flange. Also, a temperature damping unit is implemented for a reduction of the temperature variations.

[1] C. Wang, G. Thummes, C. Heiden, Cryogenics 37, 159-164 (1997)

TT 23: Magnetic Heuslers, Half-Metals, Semiconductors, and Oxides (organized by MA)

Time: Monday 15:00–18:45 Location: H 1012

TT 23.1 Mon 15:00 H 1012

The role of spin-orbit coupling and complex magnetism in the electronic structure of bulk and thin film $CaIrO_3$ — •Kerstin Dörr, Yuriy Mokrousov, Stefan Blügel, and Marjana Lezaic — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

One of the very lively research fields in condensed-matter physics is focussing on transition-metal oxides (TMO), due to a large variety of interesting physical properties they present that can be exploited in potential applications. Especially the question what drives a TMO to become insulating or metallic is an ongoing discussion, owing to the complexity of the physical effects that play a role in such systems. E.g., in well studied 3*d* compounds the enhanced onsite Coulomb repulsion drives the system into an insulating state. In contrast to this, in 5*d* TMOs the Coulomb repulsion is reduced but its interplay with the spin-orbit coupling can again force the system to become insulating, undergoing the so called spin-orbital Mott transition. In this talk we will discuss these effects in the 5*d* TMO $CaIrO_3$ in orthorhombic perovskite form. Furthermore, we will present our first-principles study of the influence of magnetism and the modifications of the bulk bandstructure of this compound in thin films.

TT 23.2 Mon 15:15 H 1012

Anisotropy of magnetic interactions in β-Li_2IrO_3 — •Alexander Yaresko and Yoshiro Nohara — MPI FKF, Stuttgart, Germany

Iridium oxides α-Li_2IrO_3 and α-Na_2IrO_3 with a honeycomb lattice attracted much attention as possible candidates for realization of a Kitaev model with bond-dependent anisotropic magnetic interactions. Recently, another complex Ir oxide β-Li_2IrO_3 has been synthesized which is expected to be close to forming a Kitaev spin liquid. Ir ions in this oxide form a "hyper-honeycomb" lattice, a three-dimensional analogue of the honeycomb lattice of α-Na_2IrO_3. We performed LDA+U band structure calculations for β-Li_2IrO_3 with different magnetic orderings of Ir magnetic moments. The results are mapped onto a model which includes isotropic Heisenberg-like as well as bond-dependent

anisotropic interactions. It is shown that the contribution of the anisotropic interactions to the magnetic energy is at least as strong as isotropic one.

TT 23.3 Mon 15:30 H 1012

Kitaev interactions in $4d_5$ honeycomb systems: Li_2RhO_3 vs $RuCl_3$ — •Ravi Yadav, Vamshi Mohan Katukuri, Satoshi Nishimoto, Liviu Hozoi, and Jeroen Van Den Brink — Institute forTheoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany

While electronic-structure calculations within either the wavefunction-based [1,2] or density functional theory [3] framework agree on the magnitude and the signs of the Kitaev couplings in $5d^5$ honeycomb iridates, much less is known on these effective exchange constants in the $4d^5$ analogues. We here discuss the outcome of many-body, wavefunction-based quantum chemistry computations for these interaction parameters in Li_2RhO_3 and $RuCl_3$. The ab initio values for the nearest-neighbor couplings, both isotropic and anisotropic, are further fed to an extended spin Hamiltonian that includes additionally 2^{nd}- plus 3^{rd}-neighbor Heisenberg terms and on the basis of exact-diagonalization calculations predictions are made for the nature of the magnetic ground states in these compounds.

[1] Vamshi M. Katukuri et al, New J. Phys. 16 (2014) 013056.
[2] Satoshi Nishimoto et al, arXiv:1403.6698.
[3] Youhei Yamaji et al, Phys. Rev. Lett. 113, 107201.

TT 23.4 Mon 15:45 H 1012

Magnetic excitations in the anomalous ferromagnetic metal $SrRuO_3$ — •Stefan Kunkemöller[1], A. Agung Nugroho[2], Yvan Sidis[3], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937, Germany — [2]Faculty of Mathematics and Natural Sciences, Jl. Ganesa 10 Bandung, 40132, Indonesia — [3]Laboratoire Léon Brillouin, CEA Saclay, F-91191 Gif sur Yvette Cedex, France

$SrRuO_3$ is the infinite-layer perovskite of the Ruddlesden-Popper series of ruthenates. It exhibits ferromagnetic ordering and highly anomalous electronic properties. At Cologne University we could recently grow several $SrRuO_3$ single-crystals with a mass of few grams each using a Canon Machinery image furnace. Inelastic neutron scattering experiments on the magnon dispersion were performed at the 2T thermal triple-axis spectrometer of the Laboratoire Léon Brillouin in Saclay. At intermediate energies and low temperature an isotropic magnon dispersion is observed as it is expected for a nearly cubic material. The magnon dispersion along the three main-symmetry directions of the pseudo-cubic material can be described by simple spin-wave theory with a gap of 1.7(2) meV and a magnetic stiffness constant of 95(5) meVÅ^2. Strong magnon-like scattering is observed till 280 K and there is no evidence for essential softening of the dispersion across the magnetic ordering in contrast to any simple Heisenberg model.

TT 23.5 Mon 16:00 H 1012

Induced magnetic monopoles on magnetoelectric surfaces — •Quintin Meier, Michael Fechner, and Nicola A. Spaldin — ETH Zürich, Department for Materials, Zürich, Switzerland

We calculate the magnetic fields caused by a point charge adjacent to the surface of a magnetoelectric, that is a material in which an electric field induces a magnetization and vice versa. The electric point charge induces monopolar and quadrupolar magnetic fields in the magnetoelectric[1]. However in the outside area the field is purely monopolar ($B \propto r^{-2}$). We show that this behaviour is valid not only for materials with isotropic magnetoelectric responses[2], but for the broader class of uniaxial magnetoelectric materials as well. Moreover, our analysis of the field strength shows that a already single charge near the prototypical uniaxial magnetoelectric, Cr_2O_3, induces a monopolar stray field which should be detectable by experiment. [1] Fechner, M. et al., Phys. Rev. B. 89, 184415 (2014) [2] Qi, X.-L. et al., Science, 323(5), 1184 (2009)

TT 23.6 Mon 16:15 H 1012

Ab initio study of the magnetic properties of Sr_2FeMoO_6 with defects — •Martin Hoffmann[1,2], Victor N. Antonov[3], Wolfram Hergert[1], Arthur Ernst[2,4], and Lev Bekenov[3] — [1]Martin Luther University Halle Wittenberg, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany — [3]Institute for Metal Physics, Kiev, Ukraine — [4]University Leipzig, Germany

We used first-principle calculations with the Korringa-Kohn-Rostoker Green function method to systematically investigate the electronic and magnetic properties of Sr_2FeMoO_6 (SFMO). We applied self-interaction correction and GGA+U to take into account the correlation effects and obtain the half-metallic nature of the material. The Curie temperature T_C was obtained from calculated magnetic exchange interactions which were used in a Monte Carlo simulation.

For a continuously increasing U parameter, SFMO became half-metallic but the T_C decreased below the reported values for bulk SFMO. We investigated possibilities to find a better agreement with experiment. This might be shortcomings in the description of the electronic structure, changes in the valency of Fe or the appearance of defects like antisite disorder and oxygen vacancies.

In addition, x-ray absorption spectra were simulated with the linear muffin-tin orbital method and compared to experimental results. A good agreement was only obtained by considering a contribution of Fe^{2+} and oxygen vacancies.

TT 23.7 Mon 16:30 H 1012

Electrical and magnetic characterization of electrospun $La_{1-x}Sr_xMnO_3$ nanowires — •Thomas Karwoth[1], Xian Lin Zeng[1], Andrew Kostrubanic[2], Michael Koblischka[1], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, Saarland University, P.O.Box 151150, D-66041 Saarbrücken, Germany — [2]Drexel University, Philadelphia, Pennsylvania 19104, USA

Nanowires of the material class $La_{1-x}Sr_xMnO_3$ with different doping levels $x = 0.2$, 0.33, 0.5 were fabricated employing a sol-gel-process via electrospinning and a subsequent thermal treatment process based on thermal gravity analysis results. Investigations by means of scanning electron microscopy revealed an average diameter of the resulting nanowires of around 220 nm and a length of more than 50 μm. The chemical phases of the samples have been confirmed via X-Ray diffraction. The nanowires are polycrystalline with a grain size of about 15-17 nm, which corresponds to the result obtained from transmission electron microscopy. Analyses of the electronic transportation properties and of the magnetoresistive effects of the nanowire samples were carried out by a four probe measurement inside a bath cryostat. Of interest are size effects and the dependence of the properties on the stoichiometry. SQUID measurements of $M(T)$ and $M(H)$ at room temperature, 77 K and 4.2 K were carried out as well, revealing the soft magnetic character of the nanowires.

TT 23.8 Mon 16:45 H 1012

High quality Yttrium Iron Garnet grown by room temperature pulsed laser deposition and subsequent annealing — •Christoph Hauser[1], Tim Richter[1], Nico Homonnay[1], Bodo Fuhrmann[2], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale) , Germany

Yttrium Iron Garnet is a room temperature ferrimagnet, which has recently gained importance due to its application in spin pumping and the investigation of the inverse spin Hall effect [1]. The linewidth and damping which can be observed in ferromagnetic resonance are typically the most important quality criteria for YIG films. Ultrathin films with very low damping constants can been grown by pulsed laser deposition [2]. We have investigated different methods of PLD growth to obtain high quality YIG thin films. Using PLD at high substrate temperature, 20 nm thick YIG films with a FMR linewidth of 12 Oe at 9.6 GHz could be obtained. Even better quality is achieved when the YIG is deposited at room temperature and subsequently annealed in an oxygen atmosphere, where we can obtain a linewidth of less than 2 Oe at 9.6 GHz. The layers show high crystalline quality and sub-nanometer surface roughness in X-ray diffraction and reflectometry. We are going to present the results of various experiments using different layer thicknesses and annealing parameters. [1]K. Uchida et al., Appl. Phys. Lett. 97, 252504 (2010) [2]d'Allivy et al., Appl. Phys. Lett. 103, 82408 (2013)

15 min. break

TT 23.9 Mon 17:15 H 1012

Magnetostriction in pulsed magnetic fields up to 70 T - the spin states in $LaCoO_3$ — •Mathias Doerr[1], Martin Rotter[2], Sergey Granovsky[1], Michael Loewenhaupt[1], and Zhaosheng S. Wang[3] — [1]TU Dresden, Institut für Festkörperphysik, D-01062 Dresden — [2]MPI for Chemical Physics of Solids, D-01187 Dresden —

[3]FZ Dresden-Rossendorf, Hochfeld-Magnetlabor, D-01314 Dresden

Magnetoelastic investigations in pulsed magnetic fields with a pulse duration of about 10 ms are still challenging. The new optical FBG method overcomes the difficulty of mechanical noise and offers a resolution in the order of 10^{-6}. As an example, the spin states in $LaCoO_3$, important for understanding of spin-dependent transport in oxides, were analyzed by longitudinal and transversal magnetostriction measurements up to 70 T. The data show a sharp magnetic transition at about 60 T accompanied by a large volume, but only small distortion effect. Supplemented by electronic energy calculations this confirms a correlated low-to-high spin (LS/HS) transition in contrast to the propagated intermediate spin-state scenario (LS-IS-HS).

TT 23.10 Mon 17:30 H 1012

Magnetic properties of the double perovskite Sr2FeOsO6: microscopic insights from ab-initio density-functional theory study — •Sudipta Kanungo[1], Binghai Yan[1,2], Martin Jansen[3], and Claudia Felser[1] — [1]Max-Planck-Institut fur Chemische Physik fester Stoffe, 01187 Dresden, Germany — [2]Max-Planck-Institut fur Physik komplexer Systeme, 01187, Dresden, Germany — [3]Max-Planck-Institut fur Festkorperforschung, 70569 Stuttgart, Germany

Using density-functional theory calculations, we investigated the electronic and magnetic properties of the ordered 3d-5d double perovskite Sr2FeOsO6, which has recently drawn attention for interesting two step antiferromagnetic (AFM) phase transitions at low temperature in experiments. The calculated effective magnetic exchange interactions reveal the importance of long-range super-super-exchange interactions in this compound. The competition between the weak ferromagnetic Os-O-Fe short-range interaction and strong AFM Os-O-Fe-O-Os long-range interaction induces strong magnetic frustration along the crystallographic c axis. This frustration is proposed to drive the magnetic phase transition between two AFM phases in the low temperature and related lattice distortion, which were observed in experiment.

[Ref: Sudipta Kanungo, Binghai Yan, Martin Jansen, and Claudia Felser; Phys. Rev. B 89,214414 (2014)]

Email: Sudipta.Kanungo@cpfs.mpg.de

TT 23.11 Mon 17:45 H 1012

Structure and magnetic interactions in Ba3-xSrxCr2O8 — •Alsu Gazizulina, Henrik Grundmann, and Andreas Schilling — Physik-Institut of University of Zurich, Zurich, Switzerland

The spin dimer systems Ba3Cr2O8 and Sr3Cr2O8 are two candidates for the Bose Einstein condensation (BEC) of magnetic quasiparticles (triplons). We have recently reported on a peculiar non-linear tuning of the magnetic interaction constant J0 in the corresponding solid solution Ba3-xSrxCr2O8 by varying the Sr content x. By performing theoretical calculations based on the crystal structure, we could well reproduce the observed variation in J0. As the critical field Hc of the triplon BEC strongly depends on the magnetic interactions in the system, we have also probed the dependency of this critical field on x. Here, we report on the observed relationship between J0(x) and Hc(x) in Ba3-xSrxCr2O8.

TT 23.12 Mon 18:00 H 1012

Investigation Of Crystal Structure, Magnetic And Transport Properties Of La2Ni(1-X)Mn(1+X)O6 (X= -0.2; 0; 0.2; 0.4; 0.6; 0.8; 1.0) — •Gizem Aslan Cansever[1,3], Franziska Scheibel[2], Mehmet Acet[2], Ergun Tasarkuyu[1], and Michael Farle[2] — [1]Mugla Sitki Kocman University, Science Faculty,48000 Mugla, Turkey — [2]Faculty of Physics, University of Duisburg-Essen, D-47057 Duisburg — [3]IFW Dresden, Institute for Solid State Research, D-01069 Dresden, Germany

La2NiMnO6 double perovskit materials show semiconductor and ferromagnetic properties which are important in terms of spintronics applications. In this study, La2Ni(1-x)Mn(1+x)O6 materials were investigated in relation to structural, electrical and magnetic properties with varying Ni and Mn concentrations. The compounds were prepared by using the sol-gel method and then heat treated in a cylindrical furnace at 1000 °C for 24 hours. The energy dispersive x-rays (EDX) analysis shows that the actual compositions of the compounds are very close to the targeted compositions and no impurity phase is present. From the analysis of x-ray diffraction data, it was observed that La2Ni1.2Mn0.8O6 and La2NiMnO6 compounds have monoclinic structure (P21/n), but the rest of the compounds exhibit the orthorhombic (Pbnm) structure. Electrical resistivity measurements show that all compunds have semiconductor behaviour. The magnetization measurements show that La2Mn2O6 incorporates both antiferromagnetic and ferromagnetic interactions. All other investigated compounds show ferromagnetic behaviour.

TT 23.13 Mon 18:15 H 1012

Neutron scattering studies of the field-induced magnetic phases of the Helimagnetic Spinel compound $ZnCr_2Se_4$. — •Alistair Cameron[1], Dmytro Inosov[1], Pavlo Portnichenko[1], Maksym Surmach[1], and Vladimir Tsurkan[2] — [1]Institut für Festkörperphysik, Technische Universität Dresden, 01069 Dresden — [2]Universität Augsburg, 16135 Augsburg

$ZnCr_2Se_4$ is a magnetoelectric compound with a cubic spinel (m3m) structure. Magnetic materials with a spinel structure present a strong opportunity to study the interplay between spin, charge and orbital degrees of freedom in a topologically frustrated environment. Particularly, those exhibiting magnetoelectric effects are of particular interest. In zero applied field, the Cr^{3+} S=3/2 moments form an incommensurate magnetic ground state with a screw structure along the (001) direction with a T_N of 20 K, which transforms into a spin spiral state in a magnetic field.

We have performed small angle neutron scattering (SANS) measurements on this spin structure for fields applied along the (100) and (110) directions. We find a field and temperature dependent structure for both field directions, with the reciprocal space propagation vector decreasing with increasing temperature and applied field, and showing a sharp jump in propagation vector across the domain selection transition. The phase diagram deduced by SANS for both field directions appear identical. In addition to investigating the AFM phase, we also probed the proposed spin nematic phase observing no SANS signal in this state, suggesting a lack of long range order.

TT 23.14 Mon 18:30 H 1012

Intrinsic resonances in the Mn spin system of ZnMnSe quantum wells — •Janina Rautert[1], Jörg Debus[1], Vitalii Yu. Ivanov[2], Sergey M. Ryabchenko[3], Andrei A. Maksimov[4], Dmitri R. Yakovlev[1,5], and Manfred Bayer[1,5] — [1]Experimentelle Physik 2, TU Dortmund, Dortmund, Germany — [2]Institute of Physics, Warsaw, Poland — [3]Institute of Physics, Kiev, Ukraine — [4]Institute of Solid State Physics, Chernogolovka, Russia — [5]Ioffe Physical-Technical Institute, St. Petersburg, Russia

Diluted magnetic semiconductors (DMS) are regarded as model structures for new types of spin electronic devices aiming at the control of the spin degree of freedom of the carriers. Although it is known that the spin-lattice interaction of the localized Mn spins is strongly accelerated by the concentration of these spins [1], a comprehensive understanding of the real mechanism of this acceleration is still missing. We observe in the stationary and time-resolved giant Zeeman energy of the exciton in ZnMnSe quantum wells a number of minima around specific magnetic fields below 10 T. These minima depend on the optical power and Mn concentration; the photoluminescence linewidth and amplitude are also affected. We propose that at these magnetic fields the levels of excited single Mn ions and quick-relaxing antiferromagnetically coupled pairs of Mn ions have anti-crossings, thus providing highly efficient magnetization relaxation. These novel results shall contribute to the understanding of spin interactions within the Mn spin system in II-VI DMS structures. [1] J. Debus et al., Phys. Rev. B 82, 085448 (2010).

TT 24: Focus Session: Functional Semiconductor Nanowires II (organized by HL)

This is the continuation of the morning session "Functional semiconductor nanowires I".

Organization: Carsten Ronning (FSU Jena), Martin Eickhoff (JLU Giessen), Tobias Voss (TU Braunschweig)

Time: Monday 15:00–18:45 Location: EW 201

Invited Talk TT 24.1 Mon 15:00 EW 201

Light-matter interaction in wire cavities - from Purcell effect to Bose-Einstein condensates — •Rüdiger Schmidt-Grund — Universität Leipzig, Inst. für Exp. Physik II, Leipzig, Germany

I will discuss effects emerging in different regimes of light-matter interaction in, basically, ZnO-based nano- and micro-wire cavities of various type. The superior crystal quality along with very smooth surfaces of that self-organized structures allows for the observation of bosonic quantum effects like parametric mixing and multi-mode bosonic final state stimulation respective Bose-Einstein condensation (BEC), which in particular benefit from the rich mode structure of such cavities.

Depending on the photonic confinement strength lasing arises gained by electron-hole plasmas [1], from coherent photonic states fed by stimulated exciton-phonon scattering [2], and from BECs of exciton-polaritons [3]. Further, lateral conformal coating with concentric distributed Bragg reflector (DBR) shells prevents lateral losses and causes Purcell enhancement of the states lifetime in typical micropillar cavities [4]. The involved photonic modes are of one-dimensional Fabry-Perot and Whispering-Gallery type. In bare wires, usually modes of only one of these types can be observed. In DBR coated nano-wire cavities, both can coexist being at the same time in the strong and weak coupling regime with the electronic system.

[1] C. Czekalla *et al*, phys. stat. sol. b **247**, 1282 (2010). [2] T. Michalsky *et al*, Appl. Phys. Lett. **105**, 211106 (2014). [3] C.P. Dietrich *et al*, Phys. Rev. B: Rapid Comm. (2015). [4] T. Jakubczy *et al*, ACS Nano **8**, 9970 (2014).

TT 24.2 Mon 15:30 EW 201

GaAs/AlGaAs core shell nanowire lasers and their integration on Si — •Sabrina Sterzl[1], Benedikt Mayer[1], Lisa Janker[1], Bernhard Loitsch[1], Gerhard Abstreiter[1,2], Christopher Gies[3], Gregor Koblmüller[1], and Jonathan Finley[1] — [1]Walter Schottky Institut and Physik Department, TU München, Garching, Germany — [2]Institute of Advanced Studies, TU München, Garching, Germany — [3]Institute for Theoretical Physics, University of Bremen, Bremen, Germany

We present lasing from individual GaAs/AlGaAs core shell nanowires (NWs) under pulsed and continuous wave (CW) optical excitation. The tailored composition profile of the NW lasers studied by photolumines- cence measurements reveals highly efficient fundamental mode lasing with emission coupling efficiencies (β) up to 0.1, ultrafast pulse emission down to 5ps as well as CW operation. Monolithic integration of the NW lasers is achieved by a universally applicable porous dielectric SiO2 reflection layer on top of the Silicon growth substrate. The SiO2 layer maintains direct contact of the NW core to the substrate and provides sufficient reflectivities for lasing operation directly on Si. The fast pulse emission found in our experiments are in good agreement with theoretical calculations predicting possible repetition rates up to 33GHz. The findings demonstrate the versatility and high functionality of the coherent on-chip NW light sources.

TT 24.3 Mon 15:45 EW 201

Time-resolved optical spectroscopy of InGaN/GaN 3D-LEDs — •Linus Krieg[1], Johannes Dühn[1], Kathrin Sebald[1], Jürgen Gutowski[1], Christian Tessarek[2], Martin Heilmann[2], Silke Christiansen[2], and Tobias Voss[3] — [1]Institute of Solid State Physics, University of Bremen — [2]Max-Planck-Institute for the Science of Light, Erlangen — [3]Institute of Semiconductor Technology, TU Braunschweig

GaN is an efficient and widely established material for optoelectronic devices, especially light-emitting diodes (LEDs). Core-shell InGaN/GaN nano- and microrod structures are supposed to further improve the efficiency and spectral range of conventional GaN-based structures leading to LEDs in the green-to-ultraviolet spectral region. Using optical spectroscopy, we perform a characterisation of self-assembled GaN micro- and nanorods with an embedded threefold InGaN quantum well (QW). The GaN rod structures were grown in a vapour-liquid-solid (VLS) growth mode. Afterwards, InGaN QWs were deposited around the rods. After using time-integrated photoluminescence measurements to analyse the concentration and homogeneity of the indium, we focus on time-resolved optical spectroscopy and determine the temperature dependent decay times. The tip of the micro- and nanorods is partly covered with a GaN pyramid. By using micro-PL measurements, we can determine the InGaN distribution on the tip as well as the impact of the GaN pyramid. Our results show a clear decrease of decay time with rising temperature and a spectral shift of the luminescence originating from the tip.

TT 24.4 Mon 16:00 EW 201

Surface functionalization and its influence on excitonic emission of ZnO nanowires — •Lisa Schade[1], Sebastian Resch[2], Sascha Creutzburg[1], Robert Röder[1], Davide Cammi[1], Siegfried R. Waldvogel[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, FSU Jena, Max-Wien-Platz 1, 07743 Jena — [2]Institut für Organische Chemie, JGU Mainz, Duesbergweg 10-14, 55128 Mainz

Semiconductor nanowires (NW) are expected to serve as a basis for next-generation high performance devices as they serve as functional and the electrical or optical connection unit for new devices with enhanced properties. This implementation has already succeeded for NW field effect transistors as well as photonic devices like LEDs, waveguides and lasers. The combination of inorganic semiconductors and organic molecules promises hybrid systems with superior functionality. Electrical and optical properties of semiconductor NWs are very sensitive to the treatment of the surface due to the high surface-to-volume ratio, thus especially the surface bound exciton becomes a dominant feature in low temperature photoluminescence spectra, indicating information about the surface properties. For that reason ZnO NWs were coated with organic molecules and photoluminescence measurements were taken before and after the functionalization. There are some anchor-groups, which are suited for functionalization: e.g. -COO-Bu_4N^+ and -Si$(C_2H_5O)_3$ allowing the link of different chains like e.g. C_6F_{12}-C_2H_4- and C_8- . Further functionality increase will be achieved by linking organic dyes for photonic devices.

TT 24.5 Mon 16:15 EW 201

Carrier dynamics in GaN-nanowire based AlN/GaN heterostructures doped with Germanium — •Nils Rosemann[1], Pascal Hille[2], Jan Müssener[2], Pascal Becker[2], María de la Mata[3], César Magén[4], Jordi Arbiol[3,5], Jörg Teubert[2], Jörg Schörmann[2], Martin Eickhoff[2], and Sangam Chatterjee[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany — [3]Institut de Ciencia de Materials de Barcelona, ICMAB-CSIC, Campus de la UAB, ES-08193 Bellaterra, CAT, Spain — [4]Laboratorio de Microscopas Avanzadas, Instituto de Nanociencia de Aragon-RAID, Universidad de Zaragoza, ES-50018 Zaragoza Spain — [5]Institucio Catalana de Recerca I Estudis Avantas (ICREA), ES-08010 Barcelona, CAT, Spain

Wide gap materials based on AlN/GaN are promising candidates for opto electronic devices in the UV-range. Here, nanowires (NWs) are of particular interest as they exhibit a significantly reduced potential for structural defects compared to bulk due to efficient strain-relaxation during the self-assembled growth. We investigate the influence of Ge doping which has a much larger covalent radius than Si or Mg on a series of AlN/GaN structures based on GaN NWs using a streak-camera setup with high spatial resolution.

TT 24.6 Mon 16:30 EW 201

Luminescence dynamics of hybrid ZnO nanowire/CdSe quantum dot structures — •Stephanie Bley[1], Friederike Albrecht[1], Michael Diez[1], Alejandra Castro-Carranza[1], Jürgen Gutowski[1], and Tobias Voss[2] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen,

Germany — [2]Institute of Semiconductor Technology , Braunschweig University of Technology, 38106 Braunschweig, Germany

The development of cheap and efficient hybrid solar cells, which show high absorption, and a fast and efficient conversion of the incident photon energy into electrical energy is of paramount interest for regenerative energy applications. To achieve that, colloidal CdSe quantum dots with different organic linker molecules were attached to ZnO nanowires to study the luminescence dynamics and the electron transfer inside these hybrid nanostructures via time-resolved photoluminescence and photoconductivity experiments. Photo-induced electron tunneling from an excited state of the QD into the nanowire becomes visible by a particular decrease of the QD decay time. This will be discussed by introducing an appropriate rate equation model. The electron tunneling is further clearly verified by a strong enhancement of the photocurrent which can be controlled by different linker molecule lengths. Further, the influence of surface oxidation on the luminescence dynamics and electron transfer will be discussed by studying polymethylmethacrylate- and polystyrene-passivated hybrid structures.

Coffee break

Invited Talk TT 24.7 Mon 17:00 EW 201

Quantum Transport in Core/Shell Semiconductor Nanowires — •Thomas Schäpers, Fabian Haas, Patrick Zellekens, Torsten Rieger, Tobias Wenz, Yusuf Günel, Önder Gül, Natalia Demarina, Mihail Lepsa, Hans Lüth, and Detlev Grützmacher — Peter Grünberg Institute (PGI- 9) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The transport properties of GaAs/InAs core/shell nanowires is investigated, where the highly conductive InAs shell is wrapped around an insulating GaAs core nanowire. At low temperatures pronounced flux periodic (h/e) magnetoconductance oscillations are observed, when the magnetic field is oriented along the nanowire axis. These very regular oscillations are explained by the formation of closed-loop quantum states in the tube-like InAs shell comprising a flux periodic energy spectrum. The magnetoconductance oscillations are even observed at temperatures as high as 50K. When the GaAs/InAs core/shell nanowire is contacted by two superconducting Nb electrodes the carrier transport is governed by phase-coherent Andreev reflection processes. Here, the observed oscillation period in the magneto-transport corresponds to half a flux quantum (h/2e).

TT 24.8 Mon 17:30 EW 201

Influence of growth parameters on electrical transport characteristics in InAs Nanowires — •Jonathan Becker[1], Stefanie Morkötter[1], Phillip Geselbracht[1], Julian Treu[1], Simon Hertenberger[1], Max Bichler[1], Gerhard Abstreiter[1,2], Jonathan J. Finley[1], and Gregor Koblmüller[1] — [1]Walter Schottky Institut und Physik Department, TU München, Garching, Germany — [2]Walter Schottky Institut and Physik Department, TU München, Garching, Germany

In this work we present recent results on the electrical transport of nominally undoped MBE grown InAs nanowires (NWs). In particular we explore the influence of growth parameters, microstructure, aspect ratio and contact metal on the electrical properties of the NWs. Four-terminal measurements on planar, back-gated NW field effect transistor (NWFET) devices revealed room-temperature mobilities ranging from 500 to 2000 cm^2/Vs and on-off ratios of $>10^3$ at 4.2K. The obtained electron densities are in the order of $10^{17}cm^{-3}$. A strong effect of the diameter and the microstructure, altered by growth parameters, on the mobility was observed. The latter was investigated by HRTEM, simulations and temperature-dependent measurements in high detail. Here, the impact of band discontinuieties induced by stacking faults and WZ/ZB crystal phase boundaries on electron scattering is evaluated.

TT 24.9 Mon 17:45 EW 201

Giant Magnetoconductance Oscillations in Hybrid Superconductor - Semiconductor Core/Shell Nanowire Devices — •Fabian Haas[1,2], Önder Gül[1,2], Haci Yusuf Günel[1,2], Hans Lüth[1,2], Torsten Rieger[1,2], Tobias Wenz[1,2], Patrick Zellekens[1,2], Mihail Lepsa[1,2], Gregory Panaitov[1,2], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institute (PGI-9 and PGI-8), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technology

In GaAs/InAs core/shell nanowires the electrons are confined in the cylindrical conductive InAs shell. In recent publications we have shown that this InAs nanotube allows the observation of h/e flux periodic oscillations in the nanowires magnetoconductance, when a magnetic field is aligned in parallel with the nanowire axis.

In this contribution, we present novel magnetotransport measurements of GaAs/InAs core/shell nanowires, this time contacted with two superconducting Nb electrodes. We observe regular $h/2e$ half-flux periodic oscillations with amplitudes in the order of e^2/h, which is larger by two orders of magnitude than observed for the h/e oscillations in a reference sample contacted with Ti/Au leads.

Phase-coherent resonant Andreev reflections at the Nb-nanowire interface, where interfering electron-hole trajectories enclose the penetrating magnetic flux, can explain these strongly enhanced oscillations as well as the $h/2e$ flux periodicity.

TT 24.10 Mon 18:00 EW 201

Heterogenous Assembly of Silicon Nanowires for Battery Applications — •Andreas Krause[1,2], Matthias Grube[1], Jan Brückner[3], Susanne Dörfler[3], Ulrike Langklotz[4], Tony Jaumann[5], Florian M. Wisser[6], Thomas Mikolajick[1,2,7], and Walter M. Weber[1,2] — [1]Namlab gGmbh, 01187 Dresden — [2]Center for Advancing Electronics Dresden (CfAED), TU Dresden — [3]Fraunhofer Institute for Material and Beam Technology (IWS), 01277 Dresden — [4]Fraunhofer Institute for Ceramic Technologies and Systems (IKTS), 01277 Dresden — [5]Chemistry of Functional Materials (IKM), Leibniz Institute for Solid State and Materials Research (IFW), Dresden — [6]Department for Inorganic Chemistry I, Dresden University of Technology, Germany — [7]Chair of Nanoelectronic Materials, Institute of Semiconductor and Microsystems Technology, TU Dresden

Silicon is a promising anode material for Lithium storage due to its high theoretical specific capacity surpassing 4200 Ah/kg, but with a large volume expansion of 400 per cent. We show innovative anode assemblies composed of a forest of free standing Si nanowires conformally integrated on a carbon fiber network. The morphology of Si nanowires allows a volume expansion and compression lowering strain incorporation. TEM micrographs of samples before and after cycling in a battery stack show the morphology change of the incorporated nanowires. A detailed electrochemical analysis is done on various samples and shows an increased stability of Si with a remaining effective capacitance above 2000 Ah/kg(Si) after 225 full charge/discharge cycles.

TT 24.11 Mon 18:15 EW 201

Monitoring cation exchange from CdSe to Ag_2Se in individual nanowires. — •Cornelius Fendler[1], August Dorn[1], Hauke Heller[2], Andreas Kornowski[2], Robert Schön[2], and Robert Blick[1] — [1]Center for Hybrid Nanostructures, Institutes of Nanostructure and Solid State Physics, University of Hamburg, Jungiusstrasse 11c, 20355 Hamburg, Germany — [2]2Institut for physical chemistry, Grindelallee 117, 20146 Hamburg

Cation exchange is a relatively simple tool to broaden the range of material compositions available in nanostructures.[1] With sufficient monitoring tools, partial cation exchange can be used to tune the material properties to desired values.[2]

In this study we investigated the correlation between the electrical conductivity and the degree of the exchange from CdSe to Ag_2Se on individuelal nanowires. We used the solution-liquid-solid (SLS) process to directly grow CdSe nanowires off bismuth thin films on Si/SiO_2-substrates. Single CdSe wires with diameters of 30 nm to 100 nm and lengths exceeding 10 μm were contacted with titanium electrodes by confocal laser lithography. The conductivity of the individual nanowires was monitored in situ during the cation exchange reaction from CdSe to Ag_2Se. At different stages of the cation exchange reaction the samples were removed from solution, the voltage-current-characteristics were measured and the material composition was determined by wavelength-dispersive X-ray spectroscopy (WDS).

[1] J.B. Rivest et al., Chem. Soc. Rev.,2013, 42, 89.
[2] A. Dorn et al., Nano Lett. 2010, 10, 3948-3951.

TT 24.12 Mon 18:30 EW 201

Charge transport along GaAs nanowires: Surface conductivity and band bending — •Stefan Korte[1], Matthias Steidl[2], Weihong Zhao[2], Werner Prost[3], Felix Lüpke[1], Vasily

Cherepanov[1], Bert Voigtländer[1], Peter Kleinschmidt[2], and Thomas Hannappel[2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology — [2]Photovoltaics Group, Institute for Physics, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [3]CeNIDE and Center for Semiconductor Technology and Optoelectronics, University of Duisburg-Essen, 47057 Duisburg, Germany

Using a multi-tip STM as nanoprober to explore the electrical transport properties of freestanding *p*-doped GaAs nanowires, we revealed a highly increased resistivity in the nanowire base, which caused bad contact to the substrate. This high resistance can be explained by a charge carrier depletion through the whole nanowire cross section due to Fermi level pinning at surface states. To explore this, Zn-doped GaAs nanowires were grown by Au-assisted metal-organic vapor-phase epitaxy (MOVPE) in the vapor-liquid-solid growth mode with different growth procedures. We measured and analyzed I/V characteristics and resistance profiles to understand the conduction mechanisms and band bending along these nanowires.

TT 25: Brownian Motion and Transport (jointly with DY, CPP)

Time: Monday 15:00–18:45 Location: BH-N 243

Invited Talk TT 25.1 Mon 15:00 BH-N 243

universal statistics of records in random sequences — •satya majumdar — cnrs, lptms, universite paris-sud, orsay, france

Records are rather common in everyday life: we are always talking of record rainfall, record temperature, records in sports and stock prices etc. When the random sequence consists of independent random variables, the record statistics is well known. In this talk, I'll discuss the record statistics in a strongly correlated random walk sequence and show that they are universal, i.e., independent of the noise (jump) distribution. Several applications and extensions will be discussed–such as the effect of a constant drift and the effect of measurement errors.

TT 25.2 Mon 15:30 BH-N 243

Three-dimensional Brownian motion of 3D-shaped particles — •Felix Höfling — Max Planck Institute for Intelligent Systems, Stuttgart, and Institute for Theoretical Physics IV, Universität Stuttgart, Germany

The three-dimensional (3D) Brownian motion of colloidal particles of general 3D-shape is considered in the overdamped limit. First for an ellipsoidal particle, the Smoluchowski equation for the joint distribution of position and orientation is solved exactly through an expansion in moments. The non-Gaussian parameter is shown to simultaneously quantify the anisotropic positional diffusion and the orientational diffusion. The results are applied further to the interpretation of scattering experiments (e.g., dynamic light scattering) on suspensions of active (self-propelled) and passive nanoparticles.

Second, a screw-like shape, paradigmatic for chiral particles, is studied which gives rise to a strong hydrodynamic coupling between rotation and translation. Coupled Langevin equations for the six degrees of freedom are used to calculate auto- and cross-correlation functions of first and second order exactly. A suitable displacement–orientation correlation is shown to display a maximum at intermediate times, from which the strength of the rotation–translation coupling can be inferred. Finally, the above findings are generalised for a hydrodynamic friction matrix of general form, which encodes an arbitrary particle shape. The analytical results are supported by numerical simulations of the corresponding stochastic equations.

TT 25.3 Mon 15:45 BH-N 243

Velocity fluctuations of Brownian particle in inhomogeneous media and driven by colored noise as a sourse of 1/f fluctuations — •Rytis Kazakevicius and Julius Ruseckas — Institute of Theoretical Physics and Astronomy, Vilnius University, A. Gostauto 12, LT-01108 Vilnius, Lithuania

Nonlinear stochastic differential equations generating signals with 1/f spectrum in a broad range of frequencies have been used so far to describe socio-economical systems [1]. We have derived such equation from Langevin equations that describe the motion of a Brownian particle in an inhomogeneous environment. The inhomogeneous environment can be a result of a linear potential affecting the Brownian particle together with the steady state heat transfer due to the difference of temperatures at the ends of the medium. The correlation of collisions between the Brownian particle and the surrounding molecules can lead to the situation where the finite correlation time becomes important, thus we have investigated the effect of colored noise in our model. Existence of colored noise leads to the additional restriction of the diffusion and exponential cut-off of the distribution of particle positions. Narrower power law part in the distribution of the particle positions results in the narrower range of frequencies where the spectrum has power law behavior.

[1] V. Gontis, J. Ruseckas and A. Kononovicius, Physica A, 389 100 (2010).

TT 25.4 Mon 16:00 BH-N 243

Hydrodynamically enforced entropic trapping of Brownian particles — •Steffen Martens[1], Arthur Straube[2], Gerhard Schmid[3], Lutz Schimansky-Geier[2], and Peter Hänggi[3] — [1]Technische Universität Berlin, Berlin, Germany — [2]Humboldt-Universität zu Berlin, Berlin, Germany — [3]Universität Augsburg, Augsburg, Germany

In small systems spatial confinement causes entropic forces that in turn implies spectacular consequences for the control for mass and charge transport. Therefore, recent efforts in theory triggered activities which allow for an approximate description that involves a reduction of dimensionality. Up to present days, the focus was on the role of conservative forces and its interplay with confinement. Within the presented work, we overcome this limitation and succeeded in considering also "magnetic field" like, so termed non-conservative forces that derive from a vector potential [S. Martens et al., *Phys. Rev. Lett.* **110**, 010601 (2013)]. A relevant application is the fluid flow across microfluidic structures where a solute of Brownian particles is subject to both, an external bias and a pressure-driven flow. Then a new phenomenon emerges; namely, the intriguing finding of identically vanishing average particle flow which is accompanied by a colossal suppression of diffusion [S. Martens et al., arXiv:1407.5673]. This entropy-induced phenomenon, which we termed *hydrodynamically enforced entropic trapping*, offers the unique opportunity to separate particles of the same size in a tunable manner [S. Martens et al.,*Eur. Phys. J. ST* **222**, 2453-2463 (2013)].

TT 25.5 Mon 16:15 BH-N 243

On the Applicability of the Caldeira-Leggett Model to Condensed Phase Vibrational Spectroscopy — •Fabian Gottwald, Sergei Ivanov, and Oliver Kühn — Institut für Physik University of Rostock, Rostock, Germany

Formulating a rigorous system-bath partitioning approach remains an open issue. In this context the famous Caldeira-Leggett (CL) model that enables quantum and classical treatment on equal footing has enjoyed popularity. Although this model is by any means useful as a theoretical tool, its validity for describing anharmonic dynamics of real systems is often taken for granted. We investigate the applicability of the model by comparing the spectra resulting from the Generalized Langevin dynamics that is based on the CL model, with their counterparts from explicit classical molecular dynamics. It is shown that the model is not able to describe real systems unless the system part of the potential is effectively harmonic. We demonstrate that it is this anharmonicity, that is at the core of all deficiencies of the model and also point out the mathematical origin of its breakdown.

15 min. break

TT 25.6 Mon 16:45 BH-N 243

Dynamics of stochatic resisitive switching — •Paul Radtke[1], Arthur Straube[1], Andrew Hazel[2], and Lutz Schimansky-Geier[1] — [1]Department of Physics, Humboldt-Universität zu Berlin, Berlin, Germany — [2]School of Mathematics, University of Manchester, Manchester, UK

Classes of dielectrics such as TiO_2 alter their resistance under the in-

fluence of an electric field or a current flowing through the system, an effect called resistive switching (RS). Thereby the resistance depends also on the past states of the system, it has a memory.

We will show how a particular one-dimensional lattice model for a bipolar device. In it, oxygen vacancies hop in between consequetive sites and thereby alter local resistances. Their dynamics governed by a Master equation with jumping rates modulated by an external electric field. We discuss the system properties and show that dynamics of the vacancies can be formulated in terms of a Burgers like equation. With its help the underlying motion of the oxygen vacancies is interpreted as nonlinear traveling waves.

TT 25.7 Mon 17:00 BH-N 243

Simulation of colloidal particles in channel geometries — •Ullrich Siems and Peter Nielaba — University of Konstanz, Germany

This talk will present the results of Brownian Dynamics Simulations of colloidal particles in external fields confined in channels. Colloidal particles are well suited model-systems for a variety of problems on different length scales, ranging from gravitational collapses over the description of pedestrians to models for atomic sized problems. In such systems confinement into channels can have a great influence on the diffusion and transport properties.

TT 25.8 Mon 17:15 BH-N 243

Nonlinear Microrheological response to a step force — •Thomas Franosch — Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Innsbruck, Austria

In a microrheological experiment the thermal or forced motion of a colloidal particle is monitored to obtain information on mechanical properties of the surroundings. While the linear response is well-characterized in terms of the fluctuation-dissipation theorem, few exact results are available for strong driving.

Here we consider the time-dependent velocity of a colloidal particle immersed in a dilute suspension of hard spheres in response to switching on a finite constant force. The dimensionless number quantifying the strength of the driving is the Péclet number $\mathrm{Pe} = F\sigma/k_BT$. We present an analytical solution exact to first order in the packing fraction. In particular, we show that at *finite times* the response is an analytic function of the Péclet number, but displays singular behavior for infinite times. Our solution technique extends the stationary state calculation [1] to the time-dependent case. The non-commutitavity of the limits $\mathrm{Pe} \to 0$ and time $t \to \infty$ is traced back to the long-time tail in the velocity-autocorrelation function due to repeated encounters with the same colloid. The scenario is strongly reminiscent of a driven particle in a lattice Lorentz model with frozen obstacles [2], and corroborates that linear response becomes qualitatively wrong at long times for arbitrarily small driving.

[1] T.M Squires and J.F. Brady, Phys. Fluids 17, 073101 (2005)
[2] S. Leitmann, T. Franosch, Phys. Rev. Lett. 111, 190603 (2013)

TT 25.9 Mon 17:30 BH-N 243

Enhancement of mobility in a feedback controlled 1D colloidal system with repulsive interactions — •Robert Gernert and Sabine H. L. Klapp — Institut für theoretische Physik, Technische Universität Berlin

Feedback control schemes are a promising way to design static and dynamic properties of colloidal suspensions [1]. In the collective transport of colloids through 1D tilted washboard potentials clusters of attractive particles are known to overcome the hindering influence of the potential barriers [2]. Here we consider a corresponding system with repulsive interactions. To enhance the mobility we propose a feedback control scheme and demonstrate its function theoretically. The control is modelled by a symmetrically confining potential, like an optical tweezer, and it is always centered around the mean particle position. For the theoretical demonstration we use Dynamical Density Functional Theory (DDFT) with ultra-soft as well as hard-core particle interactions. For either type of interaction the influence of the hindering washboard potential can be suppressed completely – corresponding to an enhancement of the mobility by several orders of magnitude. Further, in the regime of moderate amplification velocity oscillations are induced.

[1] B. Qian, D. Montiel, A. Bregull, F. Cichos, and H. Yang, Chem. Sci. 4, 1420 (2013)
[2] M. Evstigneev, S. von Gehlen, and P. Reimann, PRE 79, 011116 (2009)

TT 25.10 Mon 17:45 BH-N 243

Surface interactions of active Janus particles on a hexagonal close-packed colloidal crystal surface — •Udit Choudhury[1], John G. Gibbs[1,2], and Peer Fischer[1,3] — [1]Max Planck Institute for Intelligent Systems, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]Dept. of Physics & Astronomy, Northern Arizona University, Flagstaff, AZ 86011, USA — [3]Institute for Physical Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany

Autonomous, self-driven colloidal particles are being given greater attention in recent years due to the interesting dynamics associated with out-of-equilibrium systems. Although particle-particle interactions of active colloids, e.g. self-assembly and clustering, are beginning to be regularly studied, particle-surface interactions are less well investigated. Herein, we empirically study the surface interactions of spherical Janus-particles half-coated with Pt in the presence of hydrogen peroxide. The surface consists of close-packed 2D monolayer of hard spheres (beads). This non-planar surface thus corresponds to a periodic potential akin to a fcc (111) lattice face. In this way, the system is an analogue of surface diffusion of adatoms that possess kinetic energy. We find that as the concentration of hydrogen peroxide is increased, the effective translational diffusion also increases which is comparable to enhanced diffusion of adatoms on surfaces at higher temperatures. Rotational diffusion dictates fluctuations in the orientation of the driven bead that lead to jumps form one potential well to its nearest neighbor.

TT 25.11 Mon 18:00 BH-N 243

Charged transfer in a dynamical Landau-Zener Model: Application in QCA — •Alejandro Santana-Bonilla[1], Mirna Kramar[1], Rafael Gutierrez[1,2], and Giovanni Cuniberti[1,2] — [1]Technische Universität Dresden Faculty of Mechanical Science and Engineering Institute for Materials Sciences — [2]Max Bergmann Center of Biomaterials

The development of molecular based quantum cellular automata (mQCA) would open the possibility to low-dissipation information processing. One key parameter in the mQCA paradigm is the stability of intra-molecular charge transfer, which guarantees the association of *1* and *0* to two different charge configurations in the mQCA building cell. Especifically, a given charge configuration needs to be stable against thermal fluctuations. Also important is how the mQCA charge state reacts to an external driver with a given time-dependence. In this study we present a theoretical study based on the solution of the time-dependent Schrödinger equation to describe intra-molecular charge transfer in an effective model of an mQCA cell under the action of a time-dependent driver field and including thermal fluctuations. The model is parametrized via first-principle calculations in a toy molecular system able to catch the minimal requirements of a m-QCA cell

TT 25.12 Mon 18:15 BH-N 243

Calibration free 3D tracking of confined nanoparticles in a tunable nanofluidic slit — •Stefan Fringes, Michael Skaug, Heiko Wolf, Urs T. Dürig, and Armin W. Knoll — IBM Research, 8803 Rüschlikon, Switzerland

We investigate the behavior of nanoparticles in a nanofluidic slit with tunable confinement and spatial and temporal resolution of 10nm and 2ms, respectively. The high speed detection of the particles' X, Y and Z coordinates allows us to obtain the spatiotemporal probability distribution of individual particles and thus to study their confining potential-landscape both in lateral and vertical direction. To obtain the 3D trajectory of a nanometer-sized particle we use interferometric scattering detection (iSCAT). The method exploits the interference between the scattered wave from the particles and the highly reflective reference surface for a precise localization in vertical direction [1]. Evaluating the particle contrast for varying slit distances enables us to measure the scattering phase, amplitude, and consequently the z-position of individual particles without prior calibration of the particle contrast [2]. Precise knowledge of the nanoparticles' paths and surrounding potentials allows us to study confinement effects on Brownian motion and charge regulation at the participating interfaces. It further enables us to precisely trap and immobilize nanoparticles at a specific location on the substrate.

[1] P. Kukura et al., Nature Methods 6, 923-927 (2009).
[2] N. Mojarad et al., Optics Express 21, 8, 9377-9389 (2013).

TT 25.13 Mon 18:30 BH-N 243

Towards single molecule trapping and manipulation with dynamic temperature gradients — Marco Braun, Andreas Breg-

ulla, and •Frank Cichos — Molecular Nanophotonics Group, Universität Leipzig, Linnéstraße 5, 04103 Leipzig

Single nano-objects in solution are driven by Brownian motion which is fueled by thermal energy. These Brownian fluctuations increase in strength with increasing temperature. Therefore, it is at first glance counter intuitive to confine Brownian fluctuations with the help of elevated temperatures. In thermal nonequilibrium, however, temperature gradients induce thermo-phoretic and thermo-osmotic drifts which provide the means for single particle manipulation in solution. Here we describe experiments which use optically heated metal nanostructures to create dynamical temperature profiles in solution. These temperature profiles induce well defined thermo-phoretic drift fields and act as effective potentials for objects suspended in liquid. Combined with optical feedback mechanisms, such effective potentials can be shaped to store and manipulate single or even multiple objects in a small observation volume. The developed thermophoretic trapping system therefore paves the way for extended single molecule studies in solution or even well-controlled bi- or multi molecular interaction studies.

TT 26: Quantum Dynamics, Decoherence and Quantum Information (jointly with DY)

Time: Monday 15:00–18:30 Location: BH-N 334

TT 26.1 Mon 15:00 BH-N 334

Cooling a Magnetic Nanoisland by Spin-Polarized Currents — •Peter Nalbach[1], Jochen Brüggemann[1], Stephan Weiss[2], and Michael Thorwart[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Germany — [2]Theoretische Physik, Universität Duisburg-Essen and CENIDE, Germany

We investigate cooling of a vibrational mode of a magnetic quantum dot by a spin-polarized tunnelling charge current exploiting the magneto-mechanical coupling. The spin-polarized current polarizes the magnetic nano-island, thereby lowering its magnetic energy. At the same time, Ohmic heating increases the vibrational energy. A small magneto-mechanical coupling then permits us to remove energy from the vibrational motion and cooling is possible. We find a reduction of the vibrational energy below 50% of its equilibrium value. The lowest vibration temperature is achieved for a weak electron-vibration coupling and a comparable magneto-mechanical coupling. The cooling rate increases at first with the magneto-mechanical coupling and then saturates.

see: Phys. Rev. Lett. 113, 076602 (2014).

TT 26.2 Mon 15:15 BH-N 334

Dissipative Landau-Zener transitions with longitudinal and transversal noise — •Samaneh Javanbakht, Peter Nalbach, and Michael Thorwart — I. Institut f\"{u}r Theoretische Physik Universit\"{a}t Hamburg Jungiusstra\ss{}e 9, 20355 Hamburg

We have studied the Landau-Zener transition probability in a dissipative environment exhibiting both, longitudinal as well as transversal, noise. We employed the numerically exact quasi-adiabatic path integral as well as the approximate nonequilibrium Bloch equations. We find that transversal noise influences the Landau-Zener probability much stronger than longitudinal noise at equal temperature and system-bath coupling. Furthermore we reveal that transversal noise renormalizes the tunnel coupling independent of temperature. Finally, we observe that longitudinal and transversal noise cannot be treated independently but are correlated. This results in an unexpected dependence on the relative sign of the transversal and the longitudinal system-bath coupling.

TT 26.3 Mon 15:30 BH-N 334

Landau-Zener transitions in a bosonic bipartite quantum system — •Katharina Kopper, Ralf Blattmann, and Peter Hänggi — Universität Augsburg, D-86135 Augsburg

We study a bipartite quantum system consisting of two coupled optical micro-cavities as an analogue of the bosonic Landau-Zener setup. To account for dissipative effects we employ a Markovian master equation to describe the open system dynamics.

Within this framework we regard the time evolution of the system and its dependency on the characteristic parameters and discuss our findings.

TT 26.4 Mon 15:45 BH-N 334

Verification for quantum emulation in thermal equilibrium — •Iris Schwenk, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik - KIT , Karlsruhe

A quantum emulator is an experimental setup that mimics an interesting physical system of some relevance for physics or applications. In order to explore the reliability of a quantum emulator we analyse a system-bath setting in thermal equilibrium. Therefore we compute the reduced density matrix of the system analytically. Applying a diagrammatic approach we get a determining equation for the reduced density matrix. Using this equation we discuss restrictions of the scalability of a quantum emulator and possibilities to avoid them.

TT 26.5 Mon 16:00 BH-N 334

Fully pulse-controlled gate operations on qubit chains with always on coupling — Holger Frydrych[1], •Michael Marthaler[2], and Gernot Alber[1] — [1]Institut für Angewandte Physik, Technische Universität Darmstadt, D-64289 Darmstadt — [2]Institut für Theoretische Festkörperphysik , Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

We investigate a linear chain of qubits with strong, always-on nearest-neighbour couplings. Always-on coupling is simple to realize, but it raises the question of how to decouple the qubits. One possibility would be strong detuning, but the energy splitting of many qubits can only be changed slowly or the energy is fixed by tuning to a symmetry point which reduces decoherence.We propose a selective dynamical decoupling scheme, which is capable of dynamically suppressing any coupling in the chain as needed, by applying certain sequences of local pulses to individual qubits. We demonstrate how this pulse control can be used to implement single-qubit rotations and an entangling two-qubit gate between any neighbouring qubits in the chain. We find that high fidelities can be achieved as long as the number of permanently coupled qubits is not too large. As a specific example we discuss the concrete parameters needed to implement our proposal with superconducting flux qubits.

TT 26.6 Mon 16:15 BH-N 334

Entanglement content of non-equilibrium steady states — •Zoltán Zimborás[1] and Viktor Eisler[2] — [1]University College London, UK — [2]Eötvös University, Budapest, Hungary

We study the nonequilibrium steady state of a chain of harmonic oscillators and a chain of free fermions, resulting from an initial state where the two sides of the system are prepared at different temperatures. The steady state is constructed explicitly and the logarithmic negativity and mutual information is calculated between two adjacent segments of the chain. We find that, for the fermion chain the mutual information diverges logarithmically, while for the harmonic chain the steady-state negativity follows an area law and is a sum of contributions pertaining to left- and right-moving excitations emitted from the two reservoirs. As a particular case, we also discuss a local quench where both sides of the chain are initialized in their respective ground states.

[1] V. Eisler, Z. Zimborás, Phys. Rev. A 89, 032321 (2014)
[2] V. Eisler, Z. Zimborás, arXiv:1406.5474

TT 26.7 Mon 16:30 BH-N 334

Numerical Complexity in Non-Markovian Quantum Dynamics — •Michael Wiedmann and Jürgen T. Stockburger — Institute for Complex Quantum Systems, Ulm University, Albert-Einstein-Allee 11, D-89069 Ulm

Decoherence phenomena beyond perturbation theory are commonplace in condensed-matter physics, biophysics and strongly driven systems. The stochastic Liouville-von Neumann equation (SLN) [1] builds an exact, time-local and non-perturbative framework to tackle non-Markovian open system dynamics in these cases. In this technique the propagation of individual samples is non-unitary, the norm of quantum states is not preserved. Any resource-conscious numerical implementation faces the problem of deteriorating signal-to-noise ratios and increasing numbers of required trajectories. We present a propagation scheme that offers significant advances in sample statistics' efficiency

with emphasis on strong dephasing. Apart from transient dynamics we consider system correlation functions of steady states in equilibrium and non-equilibrium settings.

[1] J. T. Stockburger and H. Grabert, PRL 88, 170407 (2002)

15 min. break

TT 26.8 Mon 17:00 BH-N 334

Universal short-time response and formation of correlations after quantum quenches — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP), Avenida Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck- Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The short-time evolution of two distinct systems, the pump and probe experiments with semiconductor and the sudden quench of cold atoms in an optical lattice, is found to be described by the same universal response function. This analytic formula at short time scales is derived from the quantum kinetic theory approach observing that correlations need time to be formed. The influence of finite trapping potential is derived and discussed as well as Singwi-Sjølander local field corrections. The quantum kinetic equation allows to understand how two-particle correlations are formed and the screening and collective modes are build up.

K. Morawetz, Phys. Rev. B 90 (2014) 075303:
K. Morawetz, P. Lipavský, M. Schreiber, Phys. Rev. B 72 (2005) 233203:
K. Morawetz, Phys. Rev. E 66 (2002) 022103:
K. Morawetz, M. Bonitz, V. G. Morozov, G. Röpke, D. Kremp, Phys. Rev. E 63 (2001) 20102:
K. Morawetz, V. Spicka, P. Lipavský: Phys. Lett. A 246 (1998) 311:

TT 26.9 Mon 17:15 BH-N 334

Computing the Markovian dynamics of periodically driven systems — •Daniel Pagel, Andreas Alvermann, and Holger Fehske — Institut für Physik, Ernst-Moritz-Arndt-Universität, 17487 Greifswald, Germany

The dissipative dynamics of a quantum system that is weakly coupled to an environment can be studied with Markovian master equations. Solution of the master equation requires the choice of a computational basis. In this work we describe how exact diagonalization and the Floquet approach can be combined in a solution strategy for the master equation that is applicable also for periodically driven systems. For the example of strongly coupled quantum bits, where the usually employed quantum optical master equation has to be replaced by the master equation in the coupled eigenbasis, we compute the dissipative dynamics of initially entangled states and study the properties of the asymptotic state using correlation functions.

TT 26.10 Mon 17:30 BH-N 334

Non-equilibrium quantum dynamics of Gaussian states in open harmonic chains — •Thomas Motz, Jürgen T. Stockburger, and Joachim Ankerhold — Institute for complex quantum systems, Ulm University, Albert-Einstein-Allee 11, D-89069 Ulm, Germany

Strong driving in open quantum systems can reveal counterintuitive effects such as the dynamical creation of negative entropy changes [1] and entanglement between two Gaussian modes in a common reservoir [2]. The effect that dissipation and strong driving in combination can lead to specific quantum characteristics like entanglement and offers much potential for quantum information processing and the studies of mesoscopic thermodynamics. A rich tool to study dynamic effects in open systems proved to be the stochastic Liouville-von Neumann equation [3]. We avoid the stochastic sampling in our approach where the dynamics of the covariance matrix in a few-body system is directly described by a deterministic equation of motion. We apply this approach to a bipartite asymmetric system where entanglement generation and its sensitivity to the asymmetry is studied. Since the memory requirements for Gaussian states grow only quadratically with system size, our approach is also targeted at more complex settings like multiple coupled modes in a common or several separated reservoirs. Our equations of motion allow optimal control theory to be applied with ease.

[1] R. Schmidt et al., PRL 107, 130404 (2011).
[2] R. Schmidt et al., PRA 88, 052321 (2013).
[3] J. T. Stockburger and H. Grabert, PRL 88, 170407 (2002).

TT 26.11 Mon 17:45 BH-N 334

Markovianity and Consistency in closed spin lattices — •Daniel Schmidtke and Jochen Gemmer — Fachbereich Physik, Universität Osnabrück, Osnabrück, Germany

Dynamics of closed quantum systems may be mapped onto stochastic processes in case they are in accordance with conditions regarding Markovianity and Consistency. These conditions can be derived from the path measures of the Consistent Histories approach by introducing a decoherence functional and conditional transfer-probabilities. Depending on the so called memory range one distinguishes one-step, two-step, ... etc. Markovianity. To demonstrate that these conditions are indeed fulfilled in some closed quantum systems an detailed numerical investigation of spin lattices has been done by directly quantifying the negligible Non-Markovianity and negligible Non-Consistency. Though Markovianity and Consistency show very similar dependencies on, e.g., the time steps between measurements or coupling strengths within the spin system, there are no analytical proofs regarding this correlation.

TT 26.12 Mon 18:00 BH-N 334

Dynamics of the dissipative Dicke Model for a large number of atoms — •Christos Bokas, Björn Kubala, and Joachim Ankerhold — Institute for Complex Quantum Systems, Ulm University, Ulm, Germany

The Dicke Hamiltonian is used to model the coupling of a cloud of atoms to a harmonic oscillator mode. In the thermodynamic limit, a phase transition occurs when increasing the coupling strength, shifting the system from a 'normal' to a 'superradiant' state, which exhibits strong correlations between the two subsystems.

Dynamics *close to this equilibrium state* is described by the well-known Holstein-Primakov approach [1] in terms of two effective Hamiltonians containing two coupled harmonic degrees of freedom.

We aim to describe the *full coherent and dissipative dynamics* by deriving a mapping to a single effective potential valid for a large number of atoms. Starting from a highly excited atomic state, oscillations of excitations between atoms and cavity and the eventual decay to equilibrium can, hence, be studied within this approach.

[1] C. Emary and T. Brandes, Phys. Rev. E **67**, 066203 (2003).

TT 26.13 Mon 18:15 BH-N 334

Dynamics of the dissipative Dicke model: superradiance of cold atoms via a superconducting cavity — Sebastian Fuchs[1,2], •Björn Kubala[1], Miles Blencowe[3], and Joachim Ankerhold[1] — [1]Insitute for Complex Quantum Systems, Ulm University, Ulm, Germany — [2]Northwestern University, Evanston IL, USA — [3]Dartmouth College, Hanover NH, USA

Superradiance is associated with two physical effects: Firstly, the cooperative emission of radiation of a large number of excited atoms into free space in a quick, strong 'superradiant burst'. Secondly, for sufficiently strong coupling of many atoms to an electromagnetic cavity mode, modeled with the Dicke Hamiltonian, a 'superradiant phase' is found, which shows macroscopic photon occupation and atomic excitation.

The two facets of superradiance can be combined in studying the dissipative dynamics of an initially excited state of the atoms towards equilibrium. We identify and characterize the analogue of the free-space burst in this scenario, and discuss how signatures of normal or superradiant phase are observable for a mesoscopic number of atoms.

TT 27: Graphene: Theory (jointly with HL, O)

Time: Monday 15:00–17:15 Location: ER 164

TT 27.1 Mon 15:00 ER 164

The decoupling of epitaxial graphene on SiC by hydrogen intercalation: an *ab initio* study — •Lydia Nemec[1], Patrick Rinke[1,2], Volker Blum[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Aalto University, Helsinki, Fi — [3]Duke University, Durham, NC, USA

Large-scale ordered epitaxial graphene can be grown on various substrates, out of which silicon carbide (SiC) is one of the most promising. The exact material properties of graphene depend on the growth conditions and its interaction with the substrate. By hydrogen intercalation of epitaxial graphene on the Si-face of SiC the graphene layer decouples from the substrate forming quasi-free-standing monolayer graphene (QFMLG) [1].

We performed an density functional theory study of QFMLG on the polar 6H-SiC(0001) surface based on a van der Waals corrected semi-local exchange-correlation functional using the all-electron numeric atom-centered basis function code FHI-aims. We find an adsorption height in excellent agreement with X-ray standing wave experiments, a very low buckling of the graphene layer, and a very homogeneous electron density at the interface. All these features improve the electronic properties of QFMLG compared to epitaxial graphene.

Using the insight gleaned on the Si-face, we present the structure of a hypothetical QFMLG phase on the C-face of SiC. We find that hydrogen intercalation is a promising option to control the SiC-graphene interface.

[1] C. Riedl, *et. al*, PRL 103, 246804 (2009).

TT 27.2 Mon 15:15 ER 164

Two-dimensional analysis of the double-resonant 2D Raman mode in bilayer graphene — •Felix Herziger[1], Matteo Calandra[2], Paola Gava[2], Patrick May[1], Michele Lazzeri[2], Francesco Mauri[2], and Janina Maultzsch[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]IMPMC, Université Pierre et Marie Curie, CNRS, 75252 Paris, France

The double-resonant 2D-mode Raman process in bilayer graphene has been discussed controversially in recent years. In this context, different models were proposed to explain the complex lineshape observed in experiments.

Using a two-dimensional first-principles calculation, we investigate the dominant contributions to the double-resonant Raman scattering cross-section of the 2D mode in bilayer graphene [1]. In contrast to previous works, we demonstrate that so-called 'inner' processes are, by far, the most dominant processes, as in single-layer graphene. Moreover, we show that the splitting between the two TO-derived phonon branches in bilayer graphene cannot be neglected for a consistent understanding of the 2D-mode lineshape. Additionally, we investigate the contributions from both TO branches to the symmetric and antisymmetric scattering processes. Our results answer the long-standing question regarding the different contributions to the 2D-mode lineshape in bilayer graphene.

[1] F. Herziger, M. Calandra, P. Gava, P. May, M. Lazzeri, F. Mauri, and J. Maultzsch, Phys. Rev. Lett. 113, 187401 (2014)

TT 27.3 Mon 15:30 ER 164

Edge effects in the Raman spectra of atomically precise graphene nanoribbons: an ab-initio study — Marzio De Corato[1,2], •Deborah Prezzi[2], Alice Ruini[1,2], and Elisa Molinari[1,2] — [1]Department of Physics, Mathematics, and Informatics, University of Modena and Reggio Emilia, 41125 Modena, Italy — [2]CNR-Nanoscience Institute, S3 Center, 41125 Modena, Italy

Bottom-up techniques have proven successful to achieve ultra-narrow and structurally well-defined graphene nanoribbons (GNRs) [1-2], where different edge shapes and terminations can be obtained by varying the molecular precursors. In this work we perform density-functional perturbation theory calculations to investigate the vibrational properties of GNRs with cove-type edge structure and variable width, similar to those produced in Ref. 2. By comparison with other prototype systems, we show that the phonon modes and the Raman spectra of these systems strongly depend on the specific edge morphology. This is particularly evident in the acoustic region, where the Radial-Like Breathing Mode (RLBM) shows sensible changes when the edge termination is modified. This makes the Raman spectrum of these GNRs very different from the case of both carbon nanotubes and ribbons with ideal armchair or zigzag edges, where the breathing mode depends on the lateral size only. Our results are in very good agreement with recent experimental data [2].

[1] J. Cai et al., Nature (London) 466, 470 (2010). [2] A. Narita et al., Nature Chem. 6, 126 (2014).

TT 27.4 Mon 15:45 ER 164

Controlling the localization of electrons in bilayer graphene — •Maximilian Fleischmann, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

Two mutually rotated layers of graphene exhibit an electronic structure that depends profoundly on the rotation angle. The small angle regime in particular is associated with significant changes of the electronic properties of the bilayer: one finds localization on the moiré lattice and a significant reduction in the Fermi velocity near the Dirac point [1]. We investigate how the electronic properties in the small angle limit may be controlled by an external electric field directed perpendicular to the bilayer. We consider a uniform field as well as modulated fields with a period chosen to "connect" the Dirac cones of the two layers in momentum space. The latter electrostatic potentials may be realized by a proper choice of substrate. We find that electric fields can be used to control the degree of localization of the quasiparticles in the bilayer. A uniform field tends to delocalize the electron states; this effect is generally less pronounced for energies close to the Dirac point. In contrast, a modulated field favours electron localization throughout the low-energy spectrum.

[1] S. Shallcross et al., Phys. Rev. B 87, 245403, 2013.

TT 27.5 Mon 16:00 ER 164

Magnetic interactions in bilayer graphene — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

The indirect exchange interaction between magnetic impurities, known as the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, is governed by the static spin susceptibility of the host system and therefore depends sensitively on the host electronic structure. For this reason, this interaction is particularly interesting for materials in which the underlying electronic spectrum is novel, such as single layer and bilayer graphene. We investigate the RKKY interaction for bilayer graphene at zero and at finite temperature, as well as for the case in which the bilayer is biased by a perpendicular electric field. At the edge of the energy gap between the two conduction (or valence) bands at the Dirac point we find a remarkable transition in the form of the RKKY interaction. For Fermi energies on either side of the gap the interaction takes asymptotically two different forms: the oscillatory or the antiferromagnetic. We show that at the Dirac point the sign of the RKKY interaction (ferromagnetic vs anti-ferromagnetic) can be controlled by an external electric field.

TT 27.6 Mon 16:15 ER 164

Is deformed graphene described by the Dirac-Weyl equation on a curved space-time? — •Fabian Rost, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

It is well known that, at low energies, the quasiparticles of graphene are described by the wave equation of massless neutrinos: the Dirac-Weyl equation. Less well understood is whether the elastically deformed graphene can be described as the DW equation on a curved space-time as suggested in [1]. To answer this question we consider both a space-time description, and a low energy treatment derived from the tight-binding model, and compare them term by term in an expansion in the deformation tensor. We find that the low energy theory contains an infinite class of deformation-dependent terms that are absent in the space-time approach. Yet all terms present in the curved-space approach can be found in the low energy theory which follows from the tight-binding model.

[1] F. de Juan, A. Cortijo, and M.A.H. Vozmediano, *P*hys. Rev. B **76**, 165409, 2007.

TT 27.7 Mon 16:30 ER 164

Phase diagram of honeycomb lattice in Iionic-Hubbard model — •Sahar Nabavi and Morad Ebrahimkhas — Department of Science, Mahabad Branch, Islamic Azad University, Mahabad 59135, Iran

Tight binding electrons on a honeycomb lattice are described by an effective Dirac theory at low energies. An alternate ionic potential (Δ) generates a single-particle gap in the spectrum. We employ the dynamical mean field theory- iterative perturbation theory (DMFT-IPT) technique, to study the effect of on-site electron correlation (U) on energy gap of a honeycomb system. For a fixed ionic potential Δ, we find that beyond a critical value $U_{c1}(\Delta)$ massive Dirac fermions become massed and we have gapped energy bands. Further increasing U beyond $U_{c2}(\Delta)$, there will be another phase transition to the Mott insulating state. Therefore the competition between the single-particle gap parameter, Δ, and the Hubbard U between $U_{c1}(\Delta) < U < U_{c2}(\Delta)$ restores the semi-metallic nature. The width of the intermediate semi-metallic regime shrinks by increasing the ionic potential. However, at small values of Δ, there is a wide interval of U values for which the system remains semi-metal. The phase diagram and energy gap of the system are identified

TT 27.8 Mon 16:45 ER 164

Antiferromagnetic coupling of vacancies in graphene on SiO_2 — •Stephan Zimmermann[1], Sven Just[2], Marco Pratzer[2], Markus Morgenstern[2], Vladislav Kataev[1], and Bernd Büchner[1] — [1]IFW Dresden, Institute of Solid State and Materials Research, 01069 Dresden, Germany — [2]II. Institute of Physics B and JARA-FIT, RWTH Aachen, 52074 Aachen, Germany

Monolayer graphene grown by chemical vapor deposition and transferred to SiO_2 is used to introduce vacancies by Ar^+ ion bombardment at a kinetic energy of 50 eV. The density of defects visible in scanning tunneling microscopy is considerably lower than the ion fluence, implying that most of the defects are single vacancies as expected from the low ion energy. The vacancies are characterized by scanning tunneling spectroscopy on graphene and highly oriented pyrolytic graphite (HOPG). A peak close to the Dirac point is found within the local density of states of the vacancies similar to the peak found previously for vacancies on HOPG. The peak persists after air exposure up to 180 min, such that electron spin resonance (ESR) at 9.6 GHz can probe the vacancies exhibiting such a peak. After an ion flux of $10/nm^2$, we find an ESR signal corresponding to a g factor of 2.001-2.003 and a spin density of 1-2 spins/nm^2. The peak width is as small as 0.17 mT indicating exchange narrowing. Consistently, the temperature-dependent measurements reveal antiferromagnetic correlations with a Curie-Weiss temperature of -10 K. Thus, the vacancies preferentially couple antiferromagnetically, ruling out a ferromagnetic graphene monolayer at ion induced spin densities of 1-2 nm^2.

TT 27.9 Mon 17:00 ER 164

Behaviour of the edge states of the $\nu = 0$ lowest Landau level in graphene beyond SU(4)-symmetry — •Angelika Knothe[1,2] and Thierry Jolicoeur[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — [2]Université Paris Sud, CNRS, LPTMS, UMR 8626, Orsay 91405 France

The $\nu = 0$ quantum Hall state of an infinite sheet of graphene is known to exhibit various different phases when the SU(4)-symmetry of spin and valley/sublattice isospin is broken by interactions and the Zeeman-effect [1]. The situation becomes even richer when considering the edge states close to the sharp boundaries of a finite piece of graphene: Recent theoretical [2] and experimental [3] works suggest that in finite samples the properties of the spin and isospin-texture and its excitations depend on the position within the lattice with respect to its edge. With the help of numerical Hartree-Fock calculations we theoretically investigate the behaviour of the edge modes of a $\nu = 0$ quantum Hall state of graphene. In our model-Hamiltonian we account for both, the influence of SU(4)-symmetric terms and such that break the symmetry, as well as for the presence of the boundary of the lattice. In doing so, we are able to understand the behaviour of different spin and isospin configurations as compared to the phases in the bulk or the predictions of a non-interacting single-electron theory [4].

[1] M. Kharitonov, Phys. Rev. B **85**, 155439 (2012) [2] G. Murthy *et al.*, Phys. Rev. B **90**, 241410(R) (2014) [3] G. Li *et al.*, Nature Commun. **4**, 1744 (2013) [4] D. A. Abanin *et al.*, Phys. Rev. Lett. **96**, 176803 (2006)

TT 28: Poster Session on Ferroic Domain Walls - Multiferroics (jointly with DF, KR, MA)

Sponsored by NT-MDT

Part of the 3-days focus on ferroic domain walls:

Tutorial, Symposium (SYDW), and three Focused Sessions.

The goal of the poster session is to present the state of the art of the research on magnetic, ferroelectric, and multiferroic domain walls bringing interested scientist together in a stimulating environment in order to stimulate vivid topical discussions.

Time: Monday 19:00–21:00 Location: Poster C

TT 28.1 Mon 19:00 Poster C

Superdomains in $K_{0.9}Na_{0.1}NbO_3$ thin films on $NdScO_3$ substrates — •Jutta Schwarzkopf[1], Martin Schmidbauer[1], Dorothee Braun[1], Albert Kwasniewski[1], Jan Sellmann[1], and Michael Hanke[2] — [1]Leibniz Institute for Crystal Growth, Berlin, Germany — [2]Paul- Drude-Institut für Festkörperelektronik, Berlin, Germany

Incorporation of lattice strain in thin films gives rise to the creation of controlled arrays of domains and can lead to very complex domain structures. Understanding of strain induced domain formation will open the possibility to selectively influence film properties. Due to its orthorhombic symmetry (K,Na)NbO_3 films offer a large variety of ferroelectric and ferroelastic domain types. In this study $K_{0.9}Na_{0.1}NbO_3$ thin films were grown under slight compressive lattice strain on $NdScO_3$ substrates by MOCVD. Lateral PFM images of the (100) oriented films reveal bundles of ferroelectric domains along the [001] substrate direction and a width of 100-200 nm which are superimposed by ferroelastic domains forming regularly arranged herringbone patterns with a periodicity of 30 nm. The domain walls within the domain bundles are tilted alternatingly by +15° and -15° with respect to the [110] orientation of the substrate. Grazing incidence x-ray diffraction experiments have shown that adjacent superdomain bands exhibit an in-plane monoclinic lattice distortion of 0.12°. We conclude that the hierarchical structure leads to a domain formation on two scales, which effectively release the misfit strain in the film induced by the substrate.

TT 28.2 Mon 19:00 Poster C

Advanced characterization of functional ferroelectric domain walls by X-ray photoelectron emission microscopy — •Jakob Schaab[1], Ingo P. Krug[2,3], Zewu Yan[4], Edith Bourret[4], Claus M. Schneider[3], Ramamoorthy Ramesh[4,5], Manfred Fiebig[1], and Dennis Meier[1] — [1]Department of Materials, ETH Zürich — [2]Institut für Optik und Atomare Physik, TU Berlin — [3]Forschungszentrum Jülich, PGI-6 — [4]Materials Science Division, LBNL Berkeley — [5]Department of Materials Science and Engineering, UC Berkeley

The observation of anomalous electronic transport at ferroelectric domain walls and its significance for nano-electronics triggered tremendous scientific interest. To date, the transport behavior and potential barriers at domain walls have been predominantly scrutinized by scanning probes. This, however, convolutes the intrinsic electronic properties with contact resistance and inhomogeneous probe fields, so that

the detailed origin of the behavior remains obscured.

Here, we report on the capability of high-resolution X-ray photoemission electron microscopy (X-PEEM) to image and characterize ferroelectric domain walls contact-free and with nanometer resolution. In the ferroelectric semiconductor ErMnO3, we visualize ferroelectric domain walls by exploiting photo-induced charging effects and generate an electronic conduction map by analyzing the kinetic energy of photoelectrons. With this we open a pathway for non-destructive and element-specific studies of electronic and chemical domain-wall structures bypassing previous experimental limitations and significantly expanding the accessible parameter space.

TT 28.3 Mon 19:00 Poster C

Strain-induced defect-polarization coupling in $SrMnO_3$ films — •Carsten Becher[1], Laura Maurel[2], Ulrich Aschauer[1], Martin Lilienblum[1], Cesar Magen[2], Dennis Meier[1], Eric Langenberg[2], Morgan Trassin[1], Javier Blasco[3], Ingo Krug[4], Pedro Algarabel[3], Nicola Spaldin[1], Jose Pardo[2], and Manfred Fiebig[1] — [1]ETH Zürich, Zürich, Switzerland — [2]Instituto de Nanoscienciencia de Aragon, Zaragoza, Spain — [3]Departemento der Fisica de la Materia Condensada, Zaragoza, Spain — [4]Institut für Optik und Atomare Physik, Berlin, Germany

Epitaxial strain can stabilize new matter phases in thin films and is thus a degree of freedom to increase functionality. Here we demonstrate a novel polar phase in 20 nm $SrMnO_3$ films that are epitaxially grown under tensile strains by pulsed laser deposition. High resolution X-Ray diffraction and transmission electron microscopy confirm the crystalline quality of the tetragonal films. We use nonlinear optics to proof that strain induces polarity, and density functional theory to show that it simultaneously increases the concentration of oxygen vacancies. These vacancies accumulate at the polar domain walls where they establish an electrostatic barrier to electron migration. As a consequence, scanning probe microscopy shows that the electrical conductance is structured into isolated "nanocapacitors" which can be charged individually.

TT 28.4 Mon 19:00 Poster C

Raman spectroscopy for the characterization of ferroelectric materials: An Overview — •Michael Rüsing[1], Peter Mackwitz[1], Gerhard Berth[1,2], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center of Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany

Nonlinear ferroelectrics are a key material class for application in integrated optics from the high power to the single photon level. The exploitable properties range from the electro-optic effect, to large nonlinear susceptibilities and the possibility to achieve quasi-phase matching by periodic poling. But design and fabrication of devices requires an extensive knowledge on the limiting factors, such as intrinsic and extrinsic defects. Here Raman spectroscopy offers a versatile tool for characterization of material properties due to its sensitivity to a wide range of effects. This work provides an overview on performed Raman studies in various ferroelectrics, including Lithium-Niobate-Tantalate mixed crystals and KTP. Determined properties include the relative scattering tensor strengths, material composition in mixed crystals and dielectric properties. Of particular interest is the study of ferroelectric domain structures, whose behavior influenced by the presence of defects.

TT 28.5 Mon 19:00 Poster C

Laser induced poling inhibition of $LiNbO_3$ using an amorphous Si absorber — Grigoris Zisis[1], Gregorio Martinez-Jimenez[1], Yohann Franz[1], Noel Helay[1], David Grech[2], Harold Chong[2], Elisabeth Soergel[3], Anna Peacock[1], and •Sakellaris Mailis[1] — [1]Optoelectronics Research Centre, University of Southampton, Highfield, Southampton, SO17 1BJ, U.K. — [2]School of Electronic and Computer Science, University of Southampton, Highfield, Southampton SO17 1BJ, U.K. — [3]Institute of Physics, University of Bonn, Wegelerstrasse 8, 53115 Bonn, Germany

Here we demonstrate laser-induced inhibition of poling in lithium niobate by irradiating a thin absorbing layer of amorphous Si, deposited on the surface of the crystal. The absorption of a-Si in the visible range is sufficiently high to produce significant temperature gradients in the substrate causing a local change in the stoichiometry of the crystal, which in turn modifies the coercive field locally.

This arrangement enables domain engineering using readily available visible laser sources instead of costly and power limiting UV lasers which were previously used to obtain inhibition of poling in this material.

Examination of the topography and piezoresponse of the PI domains, which are formed using this laser assisted method shown a "soft" domain boundary where the domain wall is not sharp but rather consists of isolated nano-domains whose density and size is a function of the distance from the centre of the laser irradiated track.

TT 28.6 Mon 19:00 Poster C

Raman Spectroscopy and Spin-Phonon-Coupling of Multiferroic $Eu_{1-x}Ho_xMnO_3$ — •Sebastian Elsässer[1], Jean Geurts[1], Vladimir V. Glushkov[2], and Anatoly M. Balbashov[2] — [1]Exp. Phys. III, University of Würzburg, Germany — [2]Prokhorov GPI, Russian Academy of Sciences, Moscow, Russia

The revival of studies on magneto-electric (ME) effects has led to rich insights in the physics of charge and spin degrees of freedom and their mutual interaction via ME coupling [1]. One of the most extensively studied effects is the inverse Dzyaloshinskii-Moriya interaction. Hereby, the ordering of the magnetic moments leads to a lattice distortion which, in turn, can induce in a permanent electric polarization. This manifests itself in the perovskite-like rare-earth manganites $RMnO_3$. Here, the average size of the rare-earth ions R^{3+} directly influences the octahedron tilting angle. This can be used to tune the coupling between the magnetic Mn sites yielding model system for the interplay of crystalline distortion, magnetic frustration and electric polarization. In this study, R= Eu^{3+} ions are partially replaced with Ho^{3+} (<30%) to achieve the multiferroic phase. Spin-phonon-coupling (SPC) is probed by temperature-dependent Raman spectroscopy. We identify the elusive peak at 650cm^{-1} to be the $B_{3g}(1)$ mode. Upon cooling renormalisation of phonon energies due to SPC-effects starts already well above T_N. We observe that the SPC-shift is mode-specific, being strongest (up to 1%) for the $B_{2g}(1)$ and $B_{3g}(1)$, which are both octahedron breathing modes.

[1] M. Fiebig, Journal of Physics D-Applied Physics **38**, 8 (2005)

TT 28.7 Mon 19:00 Poster C

Domain walls in lithium niobate investigated by Raman spectroscopy and density functional theory — •Sergej Neufeld[1], Michael Rüsing[2], Gerhard Berth[2], Artur Zrenner[2], Wolf Gero Schmidt[1], and Simone Sanna[1] — [1]Lehrstuhl für Theoretische Physik, Universität Paderborn — [2]Department Physik, Universität Paderborn

The intensity of the Raman signal associated to different phonon modes of $LiNbO_3$ is strongly modified by the presence of ferroelectric domain boundaries [1]. The intensity modulation can be exploited to map domain structures, thus using Raman spectroscopy as a non-destructive imaging tool for the investigation of polarization-domains and domain walls [2]. Unfortunately, the origin of the modifications in the Raman signal is currently unknown. In an attempt to understand the mechanisms leading to the modification of the measured intensity, we have modeled Raman scattering efficiencies from first-principles. Thereby the Raman susceptibility tensor is calculated within the density functional theory following the approach proposed by Ghosez and co-workers [3]. The approach is validated with the TO bulk phonon modes of A_1 and E symmetry and then applied to domain boundaries. The bulk Raman intensities calculated for all possible combinations of the polarization of incoming and scattered photons are in good agreement with the measured spectra. Results for simplified domain wall models are presented and discussed. [1]P. S. Zelenovskiy et. al., Appl. Phys. A 99, 741 (2010). [2]G. Berth et al., Ferroelectrics 420, 44 (2011). [3]M. Veithen et al., Phys. Rev. B 71, 125107 (2005).

TT 28.8 Mon 19:00 Poster C

Evolution of ferroelectric domain patterns in $BaTiO_3$ at the orthorhombic ↔ tetragonal phase transition — •Thorsten Limböck and Elisabeth Soergel — Institute of Physics, University of Bonn, Nussallèe 12, 53115 Bonn, Germany

Domain patterns in barium titanate (BTO) were investigated by piezoresponse force microscopy (PFM) using a variable-temperature scanning force microscope. By analyzing the vertical and the lateral PFM images, the directions of polarization of the individual domains, i. e. 6 directions for the tetragonal and 12 for the orthorhombic phase, could be identified. The change of a domain pattern when submitting the crystal to a temperature ramp between $+20°$ and $-20°$ synchronized to the PFM scanning process, was directly monitored. Finally, the possible conversions between specific domain orientations upon heating/cooling the crystal across the phase transition were experi-

mentally confirmed.

TT 28.9 Mon 19:00 Poster C

Domain wall conductivity in gold-patterned single-crystal bulk samples using c-AFM — •Thorsten Adolphs and Elisabeth Soergel — Physikalisches Institut, Universität Bonn, Wegelerstrasse 8, 53115 Bonn

Domain wall conductivity is generally measured by c-AFM, thereby applying moderate voltages between the tip and a large-area back electrode. This technique being very attractive because of its ease of use it has, however, a couple of drawbacks: (i) the voltage applied to the tip leads to electric fields at the tip apex locally exceeding E_c. Since the displacement of a domain wall is energetically favorable (when compared to the creation of new domains), local poling predominantly takes place at the domain walls, leading to a local poling current which is also seen by c-AFM; (ii) the electrical connection between the tip and the domain wall is not reliable; and (iii) different materials of the tip and the back electrode might lead to Schottky-barrier behavior of the domain-wall current. In order to overcome these drawbacks, we propose the use of small, some μm^2-sized gold-patterns evaporated on top of the sample surface, partially connecting to the domain walls. We will present first experimental results obtained with bulk, single crystalline samples prepared for c-AFM in such a way.

TT 28.10 Mon 19:00 Poster C

Local poling at domain walls in $LiNbO_3$ crystals in connection with c-AFM measurements — •Jakob Frohnhaus and Elisabeth Soergel — Physikalisches Institut, Universität Bonn, Wegelerstrasse 8, 53115 Bonn

An electrical current localized at ferroelectric domain walls recorded by means of conductive atomic force microscopy (c-AFM) can basically have two origins: electrical conductivity of the domain wall or local poling. We show that also local poling leads to c-AFM images which cannot straightforwardly be distinguished from those c-AFM images displaying the electrical conductivity of the domain wall.

TT 28.11 Mon 19:00 Poster C

Signature of domain walls in PFM measurements — •Tim Flatten and Elisabeth Soergel — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn

Piezoresponse force microscopy (PFM) is at present the technique the most used for mapping ferroelectric domain patterns. However, the unambiguous determination of the direction of polarization of the individual domains based on PFM-images is generally not straightforward. Not only the careful analysis of a set of vertical- and lateral-PFM images are required, but possibly also a set of images after the rotation of the sample by 90° are necessary for fully determining the domain pattern. In addition to the PFM-signal obtained on top of the domain faces, on might, however, also make use of the signature of the domain walls (DW) in the PFM-signal. For ↑↓ domain walls the PFM-signal shows a symmetric, tangent-like transition between the two domains. This transition, however, should exhibit different features depending on the direction of polarization of the domains adjacent to the DW and the inclination angle of the DW relative to the sample surface. Using this additional information, the full determination of the domain pattern should be facilitated.

TT 28.12 Mon 19:00 Poster C

Measurement system for the magnetoelectric effect — •Ulrich Straube and Kathrin Doerr — Martin-Luther-University Halle, Institute of Physics, FoG, Von-Danckelmann-Platz 3, 06120 Halle, Germany

Magnetoelectric materials have different and frequency-dependent magnetoelectric effects. The correct determination of these effects is difficult because of various problems including electric and magnetic shielding, sample preparation and pretreatment. A simple measurement arrangement containing a Helmholtz coil, a pair of NdFeB permanent magnets and a special preamplifier is presented. Some results obtained from magnetoelectric ceramic materials are shown.

TT 28.13 Mon 19:00 Poster C

The magnetoelectric effect across scales — •Doru C. Lupascu[1], Heiko Wende[2], Jörg Schröder[3], Matthias Labusch[3], Morad Etier[1], Ahmadshah Nazrabi[1], Irina Anusca[1], Harsh Trivedi[1], Yanling Gao[1], Marianela Escobar[1], Vladimir V. Shvartsman[1], Joachim Landers[2], Soma Salamon[2], and Carolin Schmitz-Antoniak[4] — [1]Materials Science & Center for Nanointegration Duisburg-Essen (CENIDE) — [2]Faculty of Physics & CENIDE — [3]Institute of Mechanics, all at University of Duisburg-Essen — [4]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich

Magnetoelectric coupling can arise in intrinsic multiferroics as well as composites. We will outline how for intrinsic BiFeO3 nanoparticles yield different magnetoelectric properties at room temperature than larger grains or bulk material. Magnetoelectric nanoscale composites of $BaTiO_3$ and $CoFe_2O_4$ display rather poor magnetoelectric coupling macroscopically. Their micron scale counterparts on the other hand yield nice macroscopic response. The mechanical, electrical, and magnetic effects are analyzed using techniques including Mössbauer spectroscopy, magnetic force microscopy, piezoforce microscopy, and macroscopic techniques. It will be shown that microscopic coupling is strong also for (partly) conducting magnetic inclusions and nanosystems while macroscopic properties are highly dependent on good insulation of the samples. Experimental asymmetries in determining the magnetoelectric coupling coefficient are discussed.

Support via FP7 Marie Curie Initial Training Network *Nanomotion* (grant n° 290158) & Forschergruppe 1509 are acknowledged.

TT 28.14 Mon 19:00 Poster C

Insitu X-ray studies of mechanical coupling at piezoelectric/magnetostrictive interfaces — •Philipp Jordt[1], Stjepan Hrkac[1], Olaf M. Magnussen[1,2], and Bridget M. Murphy[1,2] — [1]Institut für Experimentelle und Angewandte Physik, ChristianAlbrechts-Universität zu Kiel, Germany — [2]Ruprecht Haensel Laboratory, Christian-Albrechts-Universität zu Kiel, Germany

To optimize magnetoelectric composites for magnetic sensor applications it is necessary to understand the coupling at the interface between a piezoelectric and a magnetostrictive material. To study the coupling at the interface, we measure the lattice deformation of the piezoelectric substrate *insitu* by grazing incidence X-ray diffraction in an external magnetic field and for different thicknesses of the magnetostrictive layer grown by magnetron sputtering, using the high resolution and high intensity X-ray beam provided by Petra III (P08). We investigate the magnetic field induced strain of $(Fe_{90}Co_{10})_{78}Si_{12}B_{10}$ on ZnO and InP substrates. From the Bragg peak positions we determined the interplanar spacings in the substrates and the corresponding strain as a function of the applied magnetic field. We measure the strain for different thicknesses and get a critical thickness for the magnetostrictive layer. We thanks the DPG for funding through PAK 902.

TT 28.15 Mon 19:00 Poster C

Influence of piezoelectric induced strain on the Raman spectra of $BiFeO_3$ films — •Cameliu Himcinschi[1], Andreas Talkenberger[1], Jens Kortus[1], Alexander Schmid[2], Er-Jia Guo[3,4], and Kathrin Dörr[3,4] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg, Germany — [2]TU Bergakademie Freiberg, Institute of Applied Physics, D-09596 Freiberg, Germany — [3]Institute for Physics, Martin-Luther-University Halle-Wittenberg, 06099 Halle, Germany — [4]Institute for Metallic Materials, IFW Dresden, 01069 Dresden, Germany

$BiFeO_3$ epitaxial thin films were deposited on piezoelectric $0.72Pb(Mg_{1/3}Nb_{2/3})O_3$-$0.28PbTiO_3$ (PMN-PT) substrates with a conductive buffer layer ($La_{0.7}Sr_{0.3}MnO_3$, or $SrRuO_3$) using pulsed laser deposition. The calibration of the strain values induced by the applied voltage on the piezoelectric PMN-PT substrates was realised using X-Ray Diffraction measurements. Raman spectra monitoring as a function of the applied voltage (and hence strain) was performed in resonant conditions, using the 442 nm line of a HeCd laser. The piezoelectric induced strain in the $BiFeO_3$ films causes shifts in the phonon position. The method of piezoelectrically induced strain allows to obtain a quantitative correlation between strain and the shift of the Raman-active phonons, ruling out the influence of extrinsic factors, as growth conditions, crystalline quality of substrates, or film thickness.
This work is supported by the German Research Foundation DFG HI 1534/1-2.

TT 28.16 Mon 19:00 Poster C

Control of the magnetic properties of magnetostrictive thin films by crossing the phase transition on a Mott insulator — S. Finizio[1], A. Fantini[1,2], •T. Lenz[1], M.V. Khanjani[1], S. Altendorf[2,3], D. Passarello[2], S.S.P. Parkin[2], and M. Kläui[1] — [1]Institut für Physik, Universität Mainz, Mainz, Germany — [2]IBM Almaden Research Center, San Jose, CA, USA — [3]Max-Planck-Institut

für Mikrostrukturphysik, Halle, Germany

The study of strongly correlated materials such as the Mott insulator VO_2 has recently attracted interest, due to the possibility of manipulating materials properties on ultrafast timescales. VO_2, in particular, has been object of attention as a metal-insulator-transition (MIT) from an insulating monoclinic phase to a conducting rutile phase occurs at accessible temperatures just above RT. These changes in crystalline order within the MIT induce strain at the interface. Combined with magnetostrictive materials such as Ni, the MIT of VO_2 is exploited to study the dynamics of the magneto-elastic coupling. Here, we present MOKE and SQUID magnetometry studies of the influence of the MIT of VO_2 on the magnetic properties of a Ni thin film. VO_2 thin films were heteroepitaxially deposited by pulsed-laser-deposition on (100) TiO_2 substrates, onto which Ni film were deposited by thermal evaporation. The magnetic properties of the Ni thin films were then determined upon thermally crossing the MIT. Our results show that strong changes in the magnetic anisotropy of the Ni films occur upon crossing the MIT leading to changes in the switching fields and characteristics as needed for ultra-fast strain-induced switching.

TT 28.17 Mon 19:00 Poster C

Structural investigation of erythrosiderites by single crystal X-ray diffraction — •Tobias Fröhlich[1], Ladislav Bohatý[2], Petra Becker[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Kristallographie, Universität zu Köln

Erythrosiderites $A_2[FeX_5(H_2O)]$, where A stands for an alkali metal or ammonium ion and X for a halide ion, are antiferromagnets with Néel-temperatures ranging from 6 to 23 K [1]. This family of compounds allows to investigate the impact of structural parameters on the magnetoelectric properties by comparing their closely related structures. The compound $(NH_4)_2[FeCl_5(H_2O)]$ was found to be multiferroic with strong magnetoelectric coupling [2]. While most structures of erythrosiderites crystallize in the space group Pnma, $Cs_2[FeCl_5(H_2O)]$ structurally deviates from the other erythrosiderides and crystallizes in space group Cmcm [3]. The structures of $(NH_4)_2[FeCl_5(H_2O)]$ and $Cs_2[FeCl_5(H_2O)]$ are investigated by single-crystal X-ray diffraction. Additionally, the non-magnetic compound $(NH_4)_2[InCl_5(H_2O)]$ is structurally investigated. Irrespective the absence of magnetism, its crystal structure is very similar to that of $(NH_4)_2[FeCl_5(H_2O)]$, therefore it can be used as a reference material to separate magnetoelectric effects.

[1] J. Luzón et al., Physical Review B, **78**, 054414 (2008). [2] M. Ackermann, D. Brüning, T. Lorenz, P. Becker, L. Bohatý, New Journal of Physics **15**, 123001 (2013). [3] M. Ackermann, T. Lorenz, P. Becker, L. Bohatý, J. Phys.: Condens. Matter **26**, 206002 (2014).

TT 28.18 Mon 19:00 Poster C

Multiferroic magnonics: quantum interference, dissipationless energy transport, and Majorana fermions — •Wei Chen[1], Manfred Sigrist[2], Andreas P. Schnyder[1], Peter Horsch[1], and Dirk Manske[1] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]ETH-Zurich, Zurich, Switzerland

We demonstrate the broad applications of multiferroic materials based on their noncollinear magnetic order and magnetoelectric effect. Upon mapping the noncollinear magnetic order into a spin superfluid, the magnetoelectric effect enables the electrically controlled quantum interference of spin superfluid, indicating the possibility of a room temperature SQUID-like quantum interferometer that manifests the flux quantization of electric field. Because the magnetoelectric effect enables changing the noncollinear magnetic order by electric field, we propose that applying an oscillating electric field with frequency as low as household frequency can generate a fast, coherent rotation of the magnetic order that is free from energy loss due to Gilbert damping, and can be used to deliver electricity up to the distance of long range order. At a superconductor/multiferroic interface, the noncollinear magnetic order imprints into the superconductor via $s-d$ coupling, which can produce Majorana fermions at the edge of the superconductor without the need to adjust chemical potential.

TT 28.19 Mon 19:00 Poster C

Optical properties of Sm-doped $BiFeO_3$ close to the morphotropic phase boundary — •Florian Burkert[1], Michaela Janowski[1], Xiaohang Zhang[2], Ichiro Takeuchi[2], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Department of Materials Science and Engineering, University of Maryland, College Park, Maryland 20742, USA

The perovskite $BiFeO_3$ is a rare example for a magnetoelectric multiferroic above room temperature. It has been demonstrated on $Bi_{1-x}Sm_xFeO_3$ thin films that Sm-doping drives $BiFeO_3$ towards a morphotropic phase boundary with enhanced piezoelectric properties, concomitant with a rhombohedral to pseudo-orthorhombic structural phase transition [1]. We studied the reflectance of a similar, Sm-doped $BiFeO_3$ thin film in the far-infrared range at room temperature and ambient pressure by means of FTIR spectroscopy. With increasing Sm doping, we observe changes in the phonon spectrum, especially at Sm content around $x = 0.14$, indicating the occurrence of a structural phase transition in agreement with earlier studies.

[1] I. Takeuchi et al., Appl. Phys. Lett. **92**, 202904 (2008).

TT 28.20 Mon 19:00 Poster C

Inelastic neutron scattering studies on $LuFe_2O_4$ — •Hailey Williamson[1], Petr Čermák[3], Jörg Voigt[1], Ryoichi Kajimoto[4], Geetha Balakrishnan[2], and Manuel Angst[1] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, Germany. — [2]Department of Physics, The University of Warwick, UK. — [3]Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, Germany. — [4]Neutron Science Section, MLF Division, J-PARC Centre, Japan

Multiferroic oxides, which exhibit a coupling between magnetism and charge order (CO), constitute a strong and competitive avenue of research. The well-known $LuFe_2O_4$, the first proclaimed multiferroic through CO due to mixed valence $Fe^{2+/3+}$ bilayers separated by Lu monolayers, was initially thought to produce ferroelectricity through polarization, from the specific CO configuration within the bilayers. This fuelled intense investigation, leading to the conclusion through XMCD, bond valence sum analysis of data and macroscopic characterization, that the bilayers are charged and not polar. With much of the static crystallographic and magnetic properties uncovered, it is now essential to elucidate the dynamic properties to understand how the spin and charge are coupled. Here we present quasi-elastic magnetic scattering with a profound temperature dependence, as well as phonon dispersions at higher energies. Finally, we show an indication of a spin gap opening, on cooling through the magnetic ordering temperature.

TT 28.21 Mon 19:00 Poster C

Investigation of low-frequency Raman modes in $BiFeO_3$ epitaxial thin films with respect to azimuthal orientation — •Andreas Talkenberger[1], Cameliu Himcinschi[1], Christian Röder[1], Ionela Vrejoiu[2,3], Florian Johann[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09596 Freiberg — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle — [3]Max Planck Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart

In this work we present results of highly accurate Raman spectroscopic experiments applied in azimuthal rotation measurements on epitaxial $BiFeO_3$ thin films grown on different scandate substrates. We observe periodic changes in Raman position, full width at half maximum and intensity for some phonon modes as a function of the azimuthal angle Φ. Further analysis revealed the possibility of the so far controversial assignment of Raman modes at low frequencies (< 250 cm^{-1}) through rotational Raman measurements, that show high sensitivity towards the mentioned parameters. We successfully simulated the azimuthal behaviour of Raman intensity and position of selected modes offering a symmetry assignment for them. In addition our results support the domain character of the BFO/DSO thin film identified by piezoresponse-force microscopy measurements.

This work is supported by the German Research Foundation DFG HI 1534/1-2.

TT 28.22 Mon 19:00 Poster C

X-ray diffraction on stoichiometric YFe_2O_4 single crystals. — •Thomas Müller and Manuel Angst — Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany.

$LuFe_2O_{4-\delta}$ was long considered to be the primary example for a charge order multiferroic. $YFe_2O_{4-\delta}$ is isostructural, but the ionic radius of Y is much larger compared to Lu, leading to completely different ordering phenomena. We have grown highly stoichiometric single crystals of $YFe_2O_{4-\delta}$ by the optical floating zone method, showing for the first time 3D charge ordering in x-ray diffraction at low temperature. The phase at 200 K can be indexed using a propagation vector of $(\frac{1}{7}\frac{1}{7}\frac{9}{7})$ considering 6 twin components and second order. Likewise the 160 K

phase can be index with $q = (\frac{1}{4}\frac{1}{4}\frac{3}{4})$. While cooling not only the threefold symmetry but in contrast to $LuFe_2O_4$ also the mirror plane of the room temperature $R\bar{3}m$ structure of $YFe_2O_{4-\delta}$ are lost according to symmetry-analysis.

TT 28.23 Mon 19:00 Poster C

Photoemission electron microscopy study of two-phase Fe/$BaTiO_3$ multiferroic system — •Ashima Arora, Matteo Cialone, Akin Ünal, Sergio Valencia, and Florian Kronast — Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Str. 15, 12489 Berlin, Germany

The phenomenon of magneto-electric coupling is of great technological importance in devices such as data storage due to possible electric field control of magnetic properties. However, a single material possessing different ferroic orders which can be exploited practically is difficult to find. Therefore we study a two-phase ferroic system made up of Fe wedge on top of a $BaTiO_3$ single crystal. Here, we study the magnetization of the ferroelectric film by Photoemission Electron Microscopy (PEEM). The capability of PEEM to be element selective and sensitive to magnetic structure of the sample using the tool of X-Ray Magnetic Circular Dichroism (XMCD) makes it possible to get laterally resolved images of magnetic state for individual element in the sample. We have visualized the magnetic domains on the Fe wedge and observed that they are influenced by the BTO substrate at the bottom. In addition, the spectroscopic information using X-ray Absorption Spectroscopy (XAS) provides a deeper insight on the interplay between the ferroelectric and ferromagnetic properties at the interface of Fe and $BaTiO_3$ in the multi-ferroic system.

TT 28.24 Mon 19:00 Poster C

Towards an experimental evidence of the linear magnetoelectric coupling — •Alexander Sukhov[1], Levan Chotorlishvili[1], Paul P. Horley[2], Chenglong Jia[3], and Jamal Berakdar[1] — [1]Institut für Physik, Martin-Luther-Universität, Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Centro de Investigacion en Materiales Avanzados (CIMAV S.C.), Chihuahua/Monterrey, 31109 Chihuahua, Mexico — [3]Key Laboratory for Magnetism and Magnetic Materials of the MOE, Lanzhou University, Lanzhou 730000, China

We present a theoretical study combining simulations of ferromagnetic resonance (FMR) for interfacesof Co/$BaTiO_3$ and Fe/$BaTiO_3$ [1] and calculations of the mean first passage times for a system of single-domain Fe-nanoparticles deposited on a ferroelectric $BaTiO_3$-substrate [2]. The study is focused on the consequences of the magnetoelectric coupling - which is considered to be linear in polarization and magnetization due to a screening mechanism - on the spectra of absorbed power [1] and the mean switching times of the Fe-nanoparticles [2]. In particular, we demonstrate and discuss how to extract an information on the symmetry and the strength of the magnetoelectric coupling from FMR-experiments, which was recently evidenced in the experiments of Ref. [3] or from eventual telegraph-noise-like experiments.

[1] A. Sukhov, P.P. Horley, C.-L. Jia, J. Berakdar, J. Appl. Phys. **113**, 013908 (2013). [2] A. Sukhov, L. Chotorlishvili, P.P. Horley, C.-L. Jia, S. Mishra, J. Berakdar, J. Phys. D: Appl. Phys. **47**, 155302 (2014). [3] N. Jedrecy *at al.*, Phys. Rev. B **88**, 121409(R) (2013).

TT 28.25 Mon 19:00 Poster C

Optical investigation of ferroic domains beyond the resolution limit — •Christoph Wetli, Viktor Wegmayr, Thomas Lottermoser, and Manfred Fiebig — Department of Materials, ETH Zurich, Zurich, Switzerland

In recent years optical second harmonic generation (SHG) has been shown to be a versatile, non-destructive tool to investigate the often complex domain structures of ferroic and multiferroic materials. Ferroic domains vary broadly in structure and size, depending on the nature of the ferroic ordering. So far, however SHG was restricted to domains larger than the optical resolution limit of 1 μm. Here we present a method by applying a numerical model and simulation to overcome this limitation and to analyze ferroic domain structures some orders of magnitude smaller than the optical resolution limit.

The method is based on the relation between the orientation of the ferroic order parameter and the phase of the nonlinear optical signal. It gives a relation between domain size and density, optical resolution and the intensity of the SHG signal. To show the reliability of the model, we applied it to several simulated domain structures. The simulation of the domain structures is based on an iterative geometrical algorithm, which allows us to generate complex domain patterns like the ferroelectric vortex structures or the irregular bubble like antiferromagnetic domains in hexagonal $YMnO_3$. The numerical calculations were compared with experimental data and found to be in excellent agreement.

TT 28.26 Mon 19:00 Poster C

Emergence of ferroelectricity in multiferroic h-$YMnO_3$ — •Martin Lilienblum[1], Thomas Lottermoser[1], Sebastian Manz[1], Sverre M. Selbach[2], Andres Cano[3], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland — [2]Department of Material Science and Engineering, NTNU, N-7491 Trondheim, Norway — [3]CNRS, Université de Bordeaux, ICMCB, UPR 9048, F-33600 Pessac, France

Universal scaling laws, interfacial nano-electronics, and topological defects are currently studied using hexagonal manganites $R$$MnO_3$ (R= Sc, Y, Dy-Lu) as model system. In spite of the remarkably broad interest in the system, surprisingly little is known about the origin of the ferroelectric state. Here we solve the controversy about the emergence of the spontaneous polarization and its coupling to the underlying structural distortion by applying scanning probe microscopy (SPM) and optical second harmonic generation (SHG). We trace the spontaneous polarization by SHG from 100 K to 1450 K directly and contact-free. We find that only a single transition exists in which the polarization arises slower than expected as by-product of the structural distortion. By thermal treatments close to the structural transition and subsequent SPM scans, we show that the exceptionally robust ferroelectric domain pattern is determined only by the structural distortion. In summary we reveal that the ferroelectric order results from an interplay of electric polarization, topological effects, and temperature.

TT 28.27 Mon 19:00 Poster C

Strain-induced defect-polarization coupling in $SrMnO_3$ films — •Carsten Becher[1], Laura Maurel[2], Ulrich Aschauer[1], Martin Lilienblum[1], Cesar Magen[2], Dennis Meier[1], Eric Langenberg[2], Morgan Trassin[1], Javier Blasco[3], Ingo Krug[4], Pedro Algarabel[3], Nicola Spaldin[1], Jose Pardo[2], and Manfred Fiebig[1] — [1]ETH Zürich, Zürich, Switzerland — [2]Instituto de Nanoscienciencia de Aragon, Zaragoza, Spain — [3]Departemento der Fisica de la Materia Condensada, Zaragoza, Spain — [4]Institut für Optik und Atomare Physik, Berlin, Germany

Epitaxial strain can stabilize new matter phases in thin films and is thus a degree of freedom to increase functionality. Here we demonstrate a novel polar phase in 20 nm $SrMnO_3$ films that are epitaxially grown under tensile strains by pulsed laser deposition. High resolution X-Ray diffraction and transmission electron microscopy confirm the crystalline quality of the tetragonal films. We use nonlinear optics to proof that strain induces polarity, and density functional theory to show that it simultaneously increases the concentration of oxygen vacancies. These vacancies accumulate at the polar domain walls where they establish an electrostatic barrier to electron migration. As a consequence, scanning probe microscopy shows that the electrical conductance is structured into isolated "nanocapacitors" which can be charged individually.

TT 28.28 Mon 19:00 Poster C

Magnetoelectric domain control in multiferroic $TbMnO_3$ — •Sebastian Manz[1], Masakazu Matsubara[1,2], Masahito Mochizuki[3,4], Teresa Kubacka[1], Ayato Iyama[5], Nadir Aliouane[6], Tsuyoshi Kimura[5], Steven Johnson[1], Dennis Meier[1], and Manfred Fiebig[1] — [1]ETH Zürich — [2]Tohoku University — [3]Aoyama Gakuin University — [4]Japan Science and Technology Agency — [5]Osaka University — [6]Paul Scherrer Institute

Spin-spiral multiferroics exhibit a strong coupling between the electric and magnetic subsystems which is of potential interest for technological applications. Although these systems have been investigated for more than a decade, the magnetoelectric domain evolution under external fields is still largely unknown. Using optical second harmonic generation we resolve how electric and magnetic fields affect the multiferroic domains in the archetypal spin-spiral multiferroic $TbMnO_3$. In consecutive electric switching cycles, varying multi-domain patterns emerge before a single-domain state is obtained. This observation reflects that the domain walls can easily move without being pinned by, e.g., structural defects. In striking contrast to the electric-field response, multi-domain patterns persist when the polarization direction is flopped by applied magnetic fields. Here, a uniform polarization rotation is observed within all domains, which incorporates a transformation of neutral into nominally charged domain walls. Our results

are explained based on numerical Landau-Lifshitz-Gilbert simulations and provide first evidence for the scalability of macroscopic magneto-electric properties onto the level of domains.

TT 28.29 Mon 19:00 Poster C

Ab initio expression of magneto-electric coupling coefficients in terms of current response function — •Ronald Starke[1] and Giulio Schober[2] — [1]Institut f. Theo. Physik, Bergakademie Freiberg — [2]Institut f. Theo. Physik, Uni Heidelberg

Based on the Functional Approach to electrodynamics of media, we show that the Maxwell equations imply closed, analytical expressions of the magneto-electric coupling coefficients in terms of the current response functions. On the linear level, these expressions include all effects of inhomogeneity, anisotropy and relativistic retardation. Moreover, we relate the 36 component functions of the constitutive tensor used in the context of bi-anisotropic media to only 9 causal response functions which specify the current response to an external vector potential.

TT 28.30 Mon 19:00 Poster C

First-principles study of magnetic properties of $BaFeO_{3-\delta}$ — •Igor Maznichenko[1], Sergey Ostanin[2], Arthur Ernst[2], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Oxides with a perovskite atomic structure are ideally suited to grow two-component multiferroics, in which a ferroelectric oxide barrier is sandwiched between magnetic electrodes. For example, the perovskites $ATiO_3$ (A = Ba, Pb) can be used as ferroelectric barrier, while ferromagnetic perovskites (La,Sr)MnO_3 or $SrRuO_3$ can serve as ferromagnetic electrodes. Oxide materials are preferable in such a tunnel junction because of their compatibility and growth. Since the number of ferromagnetic conducting oxides is restricted, a search of new suitable oxide electrodes is highly desirable. Recently, the perovskite $BaFeO_3$ was reported to be ferromagnetic in bulk and as thin film [1]. Here, using a first-principles Green function method within the density functional theory, we present a study on magnetic and electronic properties of bulk $BaFeO_3$ especially focusing on the impact of structural deformations and intrinsic defects.

[1] S. Chakraverty et al., Applied Physics Letters 103, 142416 (2013).

TT 29: Focus Session: Dynamics in Many-Body Systems: Equilibration and Localization (joint session TT/DY)

Much progress has recently been made in realizing controlled and coherent many-body systems, in the fields of condensed matter as well as ultra-cold atomic systems. One of the most exciting developments in recent years is the realization that disorder and interactions together can lead to an entirely new form of localization, "many-body localization", the study of which is in its very infancy: nature, mechanism, and implications of many-body localisation are now subject of a rapidly developing field.

This Focus Session considers several aspects of many-body localisation: how to describe many-body localisation in a theoretical model; the roles of symmetry, topology, and of external driving; it also considers connections to the venerable field of Anderson localization. In addition, it features an account of recent experiments.

Organizers: Roderich Moessner and Frank Pollmann (MPI-PKS Dresden)

Time: Tuesday 9:30–13:00 Location: H 0104

Invited Talk TT 29.1 Tue 9:30 H 0104

Probing Non-Equilibrium Dynamics with Ultracold Atoms: from Quantum Magnetism to Many-Body Localization — •Immanuel Bloch — Fakultät für Physik, Ludwig Maximilians Universität, München, Germany — Max-Planck Institut für Quantenoptik, Garching b. München, Germany

Ultracold quantum gases are an ideal testbed to study non-equilibrium dynamics of closed quantum systems. Their isolation from the environment for example enables one to probe the dynamical evolution of high-energy states in strongly interacting quantum many-body system. In many of these cases, this can result in a breakdown of fundamental assumptions of statistical mechanics, leading to novel many-body paradigms such as, e.g., many-body localization. In my talk I will give several examples from recent experiments in our group where we have studied the quantum dynamics of spin-spirals in a Heisenberg ferromagnet, novel ordering phenomena in long-range interacting quantum magnets realized via Rydberg atoms and the observation of many-body localization in interacting fermionic quantum gases in disordered lattice potentials.

Invited Talk TT 29.2 Tue 10:00 H 0104

Many-Body Localization — •Dmitry Abanin — University of Geneva, Switzerland — Perimeter Institute for Theoretical Physics, Waterloo, Ontario, Canada

We are used to describing systems of many particles by statistical mechanics. However, the basic postulate of statistical mechanics – ergodicity – breaks down in so-called many-body localized systems, where disorder prevents particle transport and thermalization. In this talk, I will give an overview of recent developments in many-body localization. I will describe a phenomenological theory of the many-body localized (MBL) phase, based on new insights from quantum entanglement. I will argue that, in contrast to ergodic systems, MBL eigenstates are not highly entangled, but rather obey so-called area law, typical of ground states in gapped systems. I will use this fact to show that MBL phase is characterized by an infinite number of emergent local conservation laws, in terms of which the Hamiltonian acquires a universal form. Turning to the experimental implications, I will describe the response of an MBL systems to quenches: surprisingly, entanglement shows logarithmic in time growth, reminiscent of glasses, while local observables exhibit power-law approach to "equilibrium" values. I will support the presented theory with the results of numerical experiments, and close by discussing experimental implications and other directions in exploring ergodicity and its breaking in quantum many-body systems.

Topical Talk TT 29.3 Tue 10:30 H 0104

Long-Time Behaviour of Periodically Driven Many-Body Quantum Systems — •Achilleas Lazarides[1], Arnab Das[2], and Roderich Moessner[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Indian Association for the Cultivation of Science, Kolkata, India

We study the long-time behaviour of closed quantum systems under temporally periodic driving, arguably the simplest deviation from equilibrium. Drawing inspiration from current understanding of equilibration and thermalisation in closed quantum systems with a time-independent Hamiltonians we study the long-time behaviour of free, interacting and (many-body) localised systems under periodic driving.

15 min. break.

Topical Talk TT 29.4 Tue 11:15 H 0104

Many Body Localization and Eigenstate Order — •Shivaji Sondhi — Department of Physics, Princeton University, Princeton, NJ 08544, USA

Recent advances in our understanding of the quantum statistical mechanics of isolated quantum systems have focused attention on the properties of individual many body eigenstates of large systems. While these advances have deepened our understanding of thermal/ergodic systems, they are even more crucial for understanding the properties

of many body localized systems where statistical mechanics breaks down. In particular, as I will describe, many body localized systems can exhibit phase transitions while remaining localized wherein the properties of their eigenstates change in singular fashion even as naive statistical mechanical averages are entirely smooth.

Invited Talk TT 29.5 Tue 11:45 H 0104

Anderson Transitions and Electron-Electron Interaction — •Alexander Mirlin — Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Recent results on the interplay of Anderson localization and electron-electron-interaction effects will be reviewed.

TT 29.6 Tue 12:15 H 0104

Impact of the eigenstate thermalization hypothesis on the relaxation of significantly off-equilibrium initial states — Abdellah Khodja[1], Robin Steinigeweg[2], and •Jochen Gemmer[1] — [1]Department of Physics, University Osnabrück, Germany — [2]Institute for Theoretical Physics, Technical University Braunschweig, Germany

We investigate the connection between (a precisely stated version) of the eigenstate thermalization hypothesis (ETH) and initial state independent (ISI) equilibration of chosen observables. The focus is on a class of initial states that render the addressed observables significantly off-equilibrium, rather than on initial states contrived by quenches. An extensive numerical study on spin systems that goes beyond exact diagonalization indicates that the smallness of a certain ETH related quantity is indeed imperative to the occurence of ISI equilibration for the above class of initial states.

TT 29.7 Tue 12:30 H 0104

Typicality of Eigenstate Thermalization — •Peter Reimann — Theoretische Physik, Universität Bielefeld, Germany

Thermalization, i.e., the relaxation of a macroscopic system towards thermal equilibrium, is a very common and well-established experimental fact, but has still not been satisfacorily explained in terms of the basic laws of physics. Specifically, for isolated many-body systems, the so-called eigenstate thermalization hypothesis (ETH) has recently attracted much interest as a sufficient condition from which thermalization could be deduced. Here, this hypothesis is validated as a typicality property for the textbook example of a simple gas in a box: admitting some tiny uncertainty about the "true" value of a single model parameter, e.g. the particle interaction strength, ETH and thus thermalization are warranted for the overwheling majority of those slightly differing model parameter values.

TT 29.8 Tue 12:45 H 0104

Nonsmooth and level-resolved dynamics illustrated with a periodically driven tight binding model — •Jiang min Zhang and Masudul Haque — Max-Plank-Institute-PKS, Dresden, Germany

We point out that in the first order time-dependent perturbation theory, the transition probability may behave nonsmoothly in time and have kinks periodically. Moreover, the detailed temporal evolution can be sensitive to the exact locations of the eigenvalues in the continuum spectrum, in contrast to coarse-graining ideas. Underlying this nonsmooth and level-resolved dynamics is a simple equality about the sinc function $sinc(x) \equiv \sin x/x$. These physical effects appear in many systems with approximately equally spaced spectra, and is also robust for larger-amplitude coupling beyond the domain of perturbation theory. We use a one-dimensional periodically driven tight-binding model to illustrate these effects, both within and outside the perturbative regime.

[1] J. M. Zhang and Masudul Haque, arXiv:1404.4280.

TT 30: Correlated Electrons: Spin Systems and Itinerant Magnets – Frustrated Magnets 3 (jointly with MA)

Time: Tuesday 9:30–13:00 Location: H 0110

TT 30.1 Tue 9:30 H 0110

Collinear order in the frustrated spin-$\frac{1}{2}$ antiferromagnet $Li_2CuW_2O_8$ — •Alexander A. Tsirlin[1], Ramesh Nath[2], Kumar Ranjith[2], Deepa Kasinathan[3], and Markos Skoulatos[4] — [1]NICPB, Tallinn, Estonia — [2]Indian Institute of Science Education and Research, Trivandrum, India — [3]MPI CPfS, Dresden, Germany — [4]Laboratory of Neutron Scattering, PSI, Villigen, Switzerland

$Li_2CuW_2O_8$ is a three-dimensional spin-$\frac{1}{2}$ antiferromagnet that features collinear spin order despite abundant magnetic frustration that would normally trigger a non-collinear incommensurate order, at least on the classical level. Using density-functional calculations, we establish the spin lattice comprising two non-coplanar triangular networks that introduce frustration along all three crystallographic directions. Magnetic susceptibility and heat capacity reveal a 1D-like magnetic response, which is, however, inconsistent with the naive spin-chain model. Moreover, the high saturation field of 29 T compared to the susceptibility maximum at as low as 8.5 K give strong evidence for the importance of interchain couplings and the magnetic frustration. Below $T_N \simeq 3.9$ K, $Li_2CuW_2O_8$ develops collinear magnetic order with parallel spins along a and c and antiparallel spins along b. The ordered moment is about $0.7\,\mu_B$ according to neutron powder diffraction. This qualifies $Li_2CuW_2O_8$ as a unique three-dimensional spin-$\frac{1}{2}$ antiferromagnet, where collinear magnetic order is stabilized by quantum fluctuations.

Financial support of the Mobilitas program (ESF) is acknowledged.

TT 30.2 Tue 9:45 H 0110

Magnetism of the effective spin-1/2 compound Cs_2CoCl_4 — •Oliver Breunig[1], Markus Garst[2], Eran Sela[2], Achim Rosch[3], Benjamin Buldmann[3], Petra Becker[4], Ladislav Bohatý[4], Ralf Müller[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University — [3]Institut für Theoretische Physik, Universität zu Köln — [4]Institut für Kristallographie, Universität zu Köln

Cs_2CoCl_4 contains $CoCl_4$ tetrahedra, which form one-dimensional chains along the crystallographic b axis. The orbital groundstate of Co^{2+} ($3d^7$, S=3/2) is split by a crystal field anisotropy D into two doublets and an easy-plane anisotropy of the magnetization is established. We measured specific heat and thermal expansion at temperatures down to 50 mK and in magnetic fields applied along different crystallographic axes. At temperatures between 0.3 and 4 K a description as an effective spin-1/2 XXZ chain arises. By considering both, thermal as well as virtual excitations of higher crystal field states, we find that the spin chain is in the XY-limit with an anisotropy $J_z/J_\perp \approx 0.12$ substantially smaller than previously believed. Magnetic order arises at a field-dependent temperature $T_C(H)$ due to inter-chain couplings which form a frustrated triangular lattice. Depending on the orientation of the magnetic field we observe various ordered phases. We present phase diagrams for different field directions and discuss the origin of the phases.

TT 30.3 Tue 10:00 H 0110

Equivalence of chemical and external pressures in RCoLnO — •Giacomo Prando[1], Gianni Profeta[2], Samuele Sanna[3], Carmine Ortix[1], Rustem Khasanov[4], Anand Pal[5], Veer Awana[5], Vladislav Kataev[1], Bernd Büchner[1,6], and Roberto De Renzi[7] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany — [2]SPIN-CNR and Dipartimento di Fisica, Universitá dell'Aquila, Italia — [3]Dipartimento di Fisica, Universitá di Pavia, I-27100 Pavia, Italia — [4]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [5]National Physical Laboratory (CSIR), New Delhi, India — [6]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [7]Dipartimento di Fisica, Universitá di Parma and CNISM, Italia

We report on the local magnetic properties of the series of ferromagnetic (FM) materials RCoLnO (R = La, Pr, Nd, Sm; Ln = As, P) as investigated by means of muon spin spectroscopy under pressure P and electron spin resonance (ESR). The effect of P is shown to be quantitatively equivalent to the chemical lattice shrinkage triggered by the different ionic radii of R ions. This is verified for both experimental-dependent quantities (i. e., magnetic field at the muon site [1]) and for intrinsically material-dependent properties (i. e., FM critical tempera-

ture T_C). Results of ESR in a wide range of temperature and magnetic field clearly display that magnetism is of localized nature, despite the overall metallic behaviour of these materials.

[1] G. Prando et al., *Phys. Rev. B* **87**, 064401 (2013)

TT 30.4 Tue 10:15 H 0110

Stabilisation of the tetragonal structure in (Ba,Sr)$CuSi_2O_6$ — •Pascal Puphal[1], Natalija Van Well[1], Franz Ritter[1], Wolf Assmus[1], Denis V. Sheptyakov[2], Christian Rüegg[2,3], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-Uni. Frankfurt — [2]Lab. for Neutron Scattering and Imaging, PSI, Switzerland — [3]Dep. of Quantum Matter Physics, Uni. of Geneva, Switzerland

$BaCuSi_2O_6$ is a spin dimer system presenting a 2D Bose-Einstein condensation of triplons at low temperatures and high magnetic fields. $BaCuSi_2O_6$ undergoes a structural phase transition below 100 K into an orthorhombic structure with two different dimer layers, leading to a complex Hamiltonian. Presently, the role of frustration in the orthorhombic structure is under debate. We present results for strontium substitution on the barium side and investigate the structural transition with low temperature x-ray and neutron powder diffraction. In addition the results of magnetic and specific-heat measurements are discussed. Surprisingly, we found that already small amounts of Sr (x = 0.05) lead to a suppression of the structural phase transition and the higher symmetric tetragonal crystal structure with only one sort of Cu-dimers is stable down to lowest temperatures. With increasing Sr-content the unit cell volume decreases and the intra-dimer spacing increases. Therefore, $(Ba_{1-x}Sr_x)CuSi_2O_6$ is a spin dimer system in a well-defined tetragonal crystal structure with the possibility to control the exchange interactions. Further manipulation is possible in substituting silicon by germanium (especially considering co-substitution) resulting in an increased cell volume and intra-dimer spacing.

TT 30.5 Tue 10:30 H 0110

Non-linear bond operator theory and 1/d expansion for coupled dimer magnets — •Darshan G. Joshi and Matthias Vojta — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

For coupled-dimer Heisenberg magnets, a paradigm of magnetic quantum phase transition, we develop a systematic expansion in 1/d, where d is spatial dimension, using bond operators. We apply this technique to a model of dimers on a hyper-cubic lattice, a generalization of the square-lattice bilayer Heisenberg model to arbitrary d. We calculate physical observables at zero temperature in both the quantum paramagnetic and anti-ferromagnetic phases and show that the 1/d expansion consistently describes the entire phase diagram including the quantum critical point. In particular, we determine the dispersion and spectral-weight distribution of the elementary excitations, including the Higgs mode of the anti-ferromagnetic phase.

TT 30.6 Tue 10:45 H 0110

Magnetic properties in hexagonal iridates — •Friedrich Freund, Soham Manni, and Philipp Gegenwart — EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany

Hexagonal iridates A_2IrO_3 (A=Na or Li) are promising candidates for the realization of the Kitaev interaction, which is an anisotropic and bonding dependent interaction that can lead to novel types of spin liquid behavior. We report the synthesis, characterization and magnetic properties of poly- and single crystals of Na_2IrO_3 and two polytypes of Li_2IrO_3 [1,2]. All three materials have a threefold coordination of edge sharing IrO_6 octahedra giving rise to Kitaev exchange. While Na_2IrO_3 and α-Li_2IrO_3 form planar honeycomb layers a three-dimensional network is realized in β-Li_2IrO_3. At high temperatures, the magnetic susceptibility of all systems displays Curie-Weiss behavior with fluctuating effective 1/2 moments while at low temperatures differently ordered states are found whose properties have been investigated by neutron powder diffraction, resonant x-ray diffraction and inelastic neutron scattering [3,4].

Work in collaboration with A. Biffin, R. D. Johnson, Sungkyun Choi, A. Bombardi, P. Manuel, R. Coldea, A. Jesche and Y. Singh.

[1] Y. Singh et al., PRL **108**, 127203 (2012).
[2] T. Takayama et al., arXiv:1403.3296 (2014).
[3] A. Biffin et al., PRB **90**, 205116 (2014).
[4] S.K. Choi et al., PRL **108**, 127204 (2012).

TT 30.7 Tue 11:00 H 0110

Analysis of the optical conductivity for A_2IrO_3 (A = Na, Li) from first principles — •Ying Li[1], Kateryna Foyevtsova[2], Harald O. Jeschke[1], and Roser Valentí[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany — [2]Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada

In this talk we will present results for the optical conductivity of Na_2IrO_3 obtained within density functional theory by including spin-orbit (SO) and correlation effects (U) as implemented in GGA+SO+U. We identify the various interband transitions and show that the underlying quasi-molecular-orbital nature of the electronic structure in Na_2IrO_3 translates into distinct features in the optical conductivity. Most importantly, we will discuss that the parity of the underlying quasi-molecular orbitals built out of Iridium t2g orbitals appears to be the main factor in determining strong and weak optical transitions. We will also present optical conductivity calculations for Li_2IrO_3 and discuss the similarities and differences with Na_2IrO_3.

15 min. break.

TT 30.8 Tue 11:30 H 0110

Raman scattering on the Honeycomb Lattice Iridates A_2IrO_3 (A=Na,Li) — Vladimir Gnezdilov[1,2], Robert Bohle[1], •Peter Lemmens[1], Soham Manni[3], Friedrich Freund[3], and Philipp Gegenwart[3] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE NAS, Ukraine — [3]IP, Univ. Augsburg

Inelastic light scattering studies on single crystals of $(Na_{1-x}Li_x)_2(Ir_{1-y}Ti_y)O_3$ (x = 0, 0.1, 0.2; y = 0, 0.025) show a polarization and temperature dependent broad band as well as phonon anomalies. We discuss these observations with respect to the relevance of the Kitaev-Heisenberg model and Majorana Fermions for A_2IrO_3.

Work supported by RTG-DFG 1953/1, Metrology for Complex Nanosystems.

TT 30.9 Tue 11:45 H 0110

Magnetic heat transport in Sr_2IrO_4 — •Frank Steckel[1], Hidenori Takagi[2], Bernd Buechner[1,3], and Christian Hess[1,3] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden — [2]Max-Planck-Institute for Solid State Research, 70569 Stuttgart — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden

The layered perovskite Sr_2IrO_4 is a $5d$ transition metal oxide with an enhanced spin-orbit coupling leading to a Mott insulating ground state with $J_{\text{eff}} = \frac{1}{2}$. It exhibits canted antiferromagnetism below $T_N = 240$ K with an antiferromagnetic coupling constant of about $J = 0.1$ eV. Thermal conductivity measurements along the ab plane of a Sr_2IrO_4 single crystal provide evidence for a contribution of magnons (below T_N) to the thermal conductivity, similar to that of the isostructural 2D $S = \frac{1}{2}$ Heisenberg antiferromagnet La_2CuO_4, where a significant magnonic contribution to the heat transport is known.

TT 30.10 Tue 12:00 H 0110

Relation between structural evolution and effective Ir moments upon applied pressure during synthesis in $Ba_3YIr_2O_9$ — •Hannes Stummer, Tusharkanti Dey, Sabine Wurmehl, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research Dresden, Germany.

The intensively investigated material class of Iridium oxide based materials provides a variety of new and unknown combinations of magnetic properties with interesting novel or exotic ground states [1]. These Iridate compounds often appear in a perovskite type structure or a related derivative which are very favorable for crystal structure modifications under high pressure. High pressure synthesis therefore can be used to tune or change the magnetic properties appearing under normal pressure [2]. The Iridate $Ba_3YIr_2O_9$ crystallizes under ambient pressure synthesis in a hexagonal structure and exhibits magnetic ordering below 4 K. A synthesis pressure of 8 GPa advances the material to form a cubic double perovskite structure which is (meta-)stable at ambient pressure. For this high pressure configuration the magnetic ordering is suppressed [3]. We will present our recent results about the systematic high pressure synthesis and characterization of $Ba_3YIr_2O_9$ samples grown under different growth pressure. The main focus will be on the correlation between structural and magnetic properties depending on the applied pressure during the synthesis process.

[1] B. J. Kim et al., PRL 101, 076402 (2008).

[2] J.G. Cheng et al., PRB 88, 205114 (2013).
[3] T. Dey et al., Phys. Rev. B 88, 134425 (2013).

TT 30.11 Tue 12:15 H 0110

Propagation of the spin-orbit exciton due to the Jahn-Teller effect in systems with strong on-site spin-orbit coupling — •Ekaterina Plotnikova[1], Maria Daghofer[2], Jeroen van den Brink[1], and Krzysztof Wohlfeld[3,4] — [1]IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]University of Stuttgart Pfaffenwaldring 57 D-70550 Stuttgart — [3]Stanford University and SLAC National Accelerator Laboratory, 2575 Sand Hill Rd, Menlo Park, CA 94025 USA — [4]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland

In this work we study the interplay between the strong spin-orbit coupling and electron-phonon interaction in the strongly correlated transition metal oxides with partially filled 5d shells. We show that even relatively weak electron-phonon coupling may lead to qualitatively different physics of the 5d oxides than the one discussed so far. Thus, we derive the effective interaction between the j 'spin-orbit' coupled isospins which follows from the orbital-only interaction induced by the cooperative Jahn-Teller effect. Next, we show that such interaction may lead to a novel type of propagation of the j = 3/2 spin-orbit exciton in the ordered j = 1/2 antiferromagnet which, unlike in the pure superexchange model does not require coupling to the j =1/2 'magnon' excitations.

TT 30.12 Tue 12:30 H 0110

Anisotropic Ru^{3+} - $4d^5$ - magnetism in the α-$RuCl_3$ honeycomb system: susceptibility, specific heat and Zero field NMR — •Michael Baenitz[1], Mayukh Majumder[1], Helge Rosner[1], Alexander Tsirlin[2], Hiroshi Yasuoka[1], and Markus Schmidt[1] — [1]MPI for the Chemical Physics of Solids, 01187 Dresden, Germany — [2]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

Low dimensional 4*d*- and 5*d*-magnets show a wide variety of magnetic ground states due to crystal electric field (CEF) splitting and strong spin-orbit coupling (SOC). The Heisenberg-Kitaev model was applied for the competing bond-dependent magnetic exchange interactions in the 5*d*-honeycomb lattices (Li_2IrO_3, Na_2IrO_3). α-$RuCl_3$ turns out to be an excellent candidate for that model because the low-spin 3+ state of Ru ($4d^5$) is equivalent to the low-spin 4+ state of Ir ($5d^5$). Hexagonal α-Ru trichloride single crystals exhibit a strong magnetic anisotropy and we show that upon applying fields up to 14 T in the honeycomb plane the successive magnetic order at $T_1 = 14$ K and $T_2 = 8$ K could be completely suppressed whereas in the perpendicular direction the magnetic order is robust. Furthermore the field dependence of χ(T) implies coexisting ferro- and antiferromagnetic exchange between in-plane components of Ru^{3+}-spins, whereas for out-of-plane components a strong antiferromagnetic exchange becomes evident. ^{101}Ru zero-field nuclear magnetic resonance evidence a complex (probably chiral) long-range magnetic order below 14 K. The large orbital moment on Ru^{3+} is found in density-functional calculations.

TT 30.13 Tue 12:45 H 0110

Local and non-local correlation effects on the frustration degree in $VOMoO_4$ and Li_2VOSiO_4 — •Amin Kiani and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany

$VOMoO_4$ and Li_2VOSiO_4 are considered a realization of the two-dimensional J_1-J_2 quantum antiferromagnetic Heisenberg model. In order to study their magnetic properties we calculate the static lattice spin susceptibility $\chi(\mathbf{q}, T)$ by using the local density approximation+dynamical mean field theory (LDA+DMFT) and its cluster extension; we adopt the local vertex approximation. We show that both systems undergo a phase transition to a three-dimensional ordered state with in-plane antiferromagnetic Neel order for $VOMoO_4$ and in-plane antiferromagnetic collinear order for Li_2VOSiO_4. We extract the effective magnetic couplings from the high temperature magnetic susceptibility. For both materials we discuss the frustration degree and local and non-local correlations effects.

TT 31: Superconductivity: Fe-based Superconductors – 122 and 111

Time: Tuesday 9:30–12:45 Location: H 2053

Topical Talk TT 31.1 Tue 9:30 H 2053

Electronic Correlations in Hole- and Electron-Doped Fe-Based Superconductors and Evidence for the C_4-Magnetic Phase in $Ba_{1-x}K_xFe_2As_2$ — •Frédéric Hardy[1], Anna Böhmer[1], Thomas Wolf[1], Peter Schweiss[1], Rolf Heid[1], Robert Eder[1], Robert A. Fisher[2], and Christoph Meingast[1] — [1]IFP, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Lawrence Berkeley National Laboratory, Berkeley CA, USA

High-T_c superconductivity in the cuprates occurs at the crossover from a correlated Mott insulating state to a weaker correlated Fermi liquid as a function of doping. The Fe-pnictides were initially thought to be weakly correlated. However, we have recently shown that KFe_2As_2 is in fact highly correlated. These correlations are even further enhanced in Rb- and $CsFe_2As_2$. The temperature dependence of both the susceptibility and the thermal expansion provides strong evidence for the existence of a coherence-incoherence crossover. Whereas the correlations in the cuprates result from a large value of the Hubbard U, recent works have stressed the particular relevance of Hund's coupling J in the pnictides. Our data may be interpreted in terms of a close proximity to an orbital-selective Mott transition. We now have good thermodynamic data covering both the hole and electron doping sides of the $BaFe_2As_2$ system and we will discuss how these correlations are modified by doping. We have also re-examined in detail the underdoped region of $Ba_{1-x}K_xFe_2As_2$. We find a small region of C_4 symmetry inside the SDW state similar to that of $Na_{1-x}Ba_xFe_2As_2$. We will show how this new phase interacts with both superconductivity and SDW.

TT 31.2 Tue 10:00 H 2053

Evolution of magnetic and superconducting phases with doping and pressure in the underdoped iron-arsenide superconductor $Ba_{1-x}K_xFe_2As_2$ — •Elena Hassinger[1,2,3], Gregory Gredat[1], Fabrice Valade[1], Samuel Rene de Cotret[1], Alexandre Juneau-Fecteau[1], Jean-Philippe Reid[1], H. Kim[4], Makariy A. Tanatar[4], Ruslan Prozorov[4], B. Shen[5], H.H. Wen[5], Nicolas Doiron-Leyraud[1], and Louis Taillefer[1,2] — [1]Université de Sherbrooke, Québec, Canada — [2]Canadian Institute for Advanced Research, Toronto, Ontario, Canada — [3]Max Planck Institut für Chemische Physik fester Stoffe, Dresden, Germany — [4]Ames Laboratory, Ames, Iowa, USA — [5]Nanjing University, China

The electrical resistivity ρ of the iron-arsenide superconductor $Ba_{1-x}K_xFe_2As_2$ was measured in applied pressures up to 2.75 GPa for seven underdoped samples. Six of them are antiferromagnetic at $P = 0$ with $0.16 < x < 0.24$ and one is non-magnetic with $x = 0.26$. The stipe-like antiferromagnetic ordering temperature T_N, detected as a sharp anomaly in $\rho(T)$, decreases linearly with pressure. For every magnetic sample a second phase appears with pressure at a lower temperature T_0, which rises with pressure. The critical pressure above which this phase appears decreases with doping going to zero for $x = 0.24$ just below the critical doping for the magnetic phase. This behaviour is reminiscent of the second magnetic phase appearing in $Ba_{0.76}Na_{0.24}Fe_2As_2$ where the tetragonal symmetry is restored in favour of the scenario in which the nematic order in the iron pnictides is of magnetic origin.

TT 31.3 Tue 10:15 H 2053

Coaction of marginal Fermi liquid behavior and van Hove singularities in unconventional superconductors — •J. Fink[1,6], A. Charnukha[1], E.D.L. Rienks[2], Z.H. Liu[1], S. Thirupathaiah[1], I. Avigo[3], F. Roth[4], H.S. Jeevan[5], P. Gegenwart[5], M. Roslova[1], I. Morozov[1], S. Wurmehl[1,6], U. Bovensiepen[3], S. Borisenko[1], M. Vojta[6], and B. Büchner[1,6] — [1]IFW Dresden Germany — [2]HZB Berlin Germany — [3]Universität Duisburg-Essen Germany — [4]Center for Free-Electron Laser Science Hamburg Germany — [5]Universität Augsburg Germany — [6]TU Dresden Germany

Using ARPES we have studied the scattering rates and effective masses of the ferropnictides $(Ba/Eu)Fe_2(As_{1-x}P_x)_2$ and $NaFe_{1-x}(Co/Rh)_xAs$ as a function of the control parameter (chemical

pressure/ electron doping). The detected scattering rates of all electron and hole pockets are nearly independent of the control parameter, strongly differ for pockets having different orbital character, and are linear in energy indicating marginal Fermi liquid behavior near otimal substitution/doping. The measurements also indicate a crossing of the top of that hole pocket, having the largest scattering rate, through the Fermi level. A calculation as well as the experiments show that a coaction of marginal Fermi liquid behavior and the weakly dispersive band crossing the Fermi level leads to an extended singularity. The later can explain, possibly also in other unconventional superconductors, the strong mass enhancement near optimal doping/substitution and a superconducting phase with a small effective Fermi energy favoring a BCS-BE crossover state.

TT 31.4 Tue 10:30 H 2053

Suppressed thermal transport in Rh-doped $BaFe_2As_2$ — •Frank Steckel[1], Sheng Ran[2], Sergey L. Bud'ko[2], Paul C. Canfield[2], Bernd Buechner[1,3], and Christian Hess[1,3] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden — [2]Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden

We investigated Rh-doped $BaFe_2As_2$ by means of electrical and heat transport. The underdoped compounds show a clear suppression of phononic heat transport in the intermediate temperature regime above the structural transition temperature T_S and up to 170 K. We interprete this suppression as a strong indication towards electron-phonon coupling, spin-phonon coupling or lattice softening by nematic fluctuations above the structural transition. Additionally, strong anomalies mark the structural and superconducting transition.

TT 31.5 Tue 10:45 H 2053

Phase transitions and phase separation in undoped and Rh doped $CaFe_2As_2$ — Vladimir Gnezdilov[1,2], •Peter Lemmens[1], Yurii Pachkevich[3], Tetiana Shevtsova[3], Masataka Danura[4], Masakazu Kobayashi[4], Tasuku Mizukami[4], Kazutaka Kudo[4], and Minoru Nohara[4] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE NAS, Ukraine — [3]DonFTI, Donetsk, Ukraine — [4]Department of Physics, Okayama, Japan

Iron-pnictides Ca(Fe1-xRhx)$_2$As$_2$ (x = 0, 0.035 and 0.19) were studied across the tetragonal-orthorhombic and tetragonal collapsed tetragonal phase transitions using Raman spectroscopy. Effects of phase separation were observed in the high-temperature phase for the first time. An orbital order scenario at low temperatures for the Rh doped samples which requires a symmetry lowering down to P4/mnc or I422 without atomic displacements relative to the parent I4/mmm symmetry is discussed.

Work supported by RTG-DFG 1953/1, Metrology for Complex Nanosystems.

15 min. break.

TT 31.6 Tue 11:15 H 2053

Strain effect on the phase diagram of Ba-122 — Kazumasa Iida[1,2], •Vadim Grinenko[1], Fritz Kurth[1], Dmitriy Efremov[1], Stefan-Ludwig Drechsler[1], Marco Langer[1,3], Jan Engelmann[1], Ataru Ichinose[4], Ichiro Tsukada[4], Eike Ahrens[5], Saicharan Aswartham[1], Sabine Wurmehl[1], Ingolf Mönch[1], Manuela Erbe[1,3], Jens Hänisch[1,3], Bernhard Holzapfel[1,3], Hiroshi Ikuta[2], and Ruben Hühne[1] — [1]IFW Dresden, Germany — [2]Nagoya University, Japan — [3]Karlsruhe Institute of Technology (KIT), Germany — [4]Central Research Institute of Electric Power Industry, Nagasaka, Japan — [5]TU Dresden, Germany

Thin films offer a possibility for tuning superconducting (SC) properties without external pressure or chemical doping. In-plane strain controls the Neél temperature of the antiferromagnetic (AF) transition and the SC transition temperature or even induce superconductivity in the parent compound [1]. We studied the electronic and magnetic properties of Co, Ru, and P doped Ba-122 thin films in different strain states. We have found that the strain shifts nearly rigidly the whole phase diagram including the AF region and the SC dome in the direction of higher or lower substitution levels depending on the direction of strain (i.e. compressive or tensile). In particular, we found that the strain affects the band structure similarly as Co doping despite that the crystal structure changes differently. As a result tensile or compressive strain acts as additional *el* or *h* doping, respectively.

[1] APL **95**, 192501 (2009); **102**, 142601 (2013); Nat. Commun. **4**, 2877 (2013).

TT 31.7 Tue 11:30 H 2053

A calorimetric investigation of $RbFe_2As_2$ single crystals — •Seunghyun Khim[1], Saicharan Aswartham[1], Vadim Grinenko[1], Christian C. F. Blum[1], Frank Steckel[1], Daniel Gruner[1], Anja U. B. Wolter[1], Christian Hess[1], Stefan-Ludwig Drechsler[1], Bernd Büchner[1,2], and Sabine Wurmehl[1,2] — [1]Leibniz Institute for Solid State and Materials Research, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden, Germany

We present physical properties of single crystals of the iron pnictide superconductor $RbFe_2As_2$ grown by a self-flux method. A bulk superconducting transition at $T_c \sim 2.7$ K was consistently observed in resistivity, magnetic susceptibility and specific heat measurements. While the normal state resistivity following a T^2 dependence at low T is that of a conventional metal, the magnetic susceptibility shows a deviation from a conventional Curie-Weiss behavior and an unusual broad local maximum around 80 K. Similar humps have been observed for KFe_2As_2 and $SrCo_2As_2$. A large Sommerfeld coefficient, $\gamma_0 = 127$ mJ/mol K^2, was observed seemingly a common feature of heavily hole-doped 122 pnictides. We analyze the superconducting transition seen in our specific heat data by using the *s*-wave BCS two-gap model. The presence of a small gap is discussed as possible explanation to account for the large specific heat contribution far below T_c. The large H_{c2} anisotropy ratio, $\Gamma = H_{c2}^{ab}/H_{c2}^{c} \sim 7$ near T_c is also discussed within this multiband nature of the Fermi surface.

TT 31.8 Tue 11:45 H 2053

Detailed phase diagram of $(Ba,Na)Fe_2As_2$ — •Liran Wang[1], Anna Böhmer[1,2], Frédéric Hardy[1], Peter Schweiss[1], Thomas Wolf[1], and Christoph Meingast[1] — [1]Institute für Festkörperphysik,Karlsruher Institut für Technologie (KIT), 76344 Karlsruhe, Germany — [2]Department of Physics and Astronomy and Ames Laboratory, Iowa State University, Ames, Iowa 50011, USA

Recently a $C4$-symmetric magnetic phase has been discovered in $(Ba_{1-x}Na_x)Fe_2As_2$ [1], close to where the usual Spin Density Wave (SDW) transition disappears upon doping. Single crystal neutron diffraction showed that the spin orientation in this phase changes from in-plane in the $C2$-magnetic phase to out-of-plane [2]. Here, we reinvestigate the phase diagram of this system by closely following the doping evolution of structural, magnetic and superconducting transitions by using high-resolution thermal expansion and specific heat measurements. The resulting phase diagram is shown to be considerably more complex than previously thought [1]. Differences and similarities between the Na- and K-doped [3] systems will be discussed.

[1] Avci et al., Nature Commun. 5, 3845 (2014).
[2] F.Waβer et al., unpublished.
[3] A.Böhmer et al., unpublished.

TT 31.9 Tue 12:00 H 2053

Spin-reorientation and Excitations in $Ba_{1-x}Na_xFe_2As_2$ — •Florian Wasser[1], Sabine Wurmehl[2], Saicharan Aswartham[2], Yvan Sidis[3], Astrid Schneidewind[4,5], Jitae Park[5], Bernd Büchner[2], and Markus Braden[1] — [1]II. Physikalisches Institut, D-50937 Köln, Germany — [2]Institute for Solid State Research, D-01171 Dresden, Germany — [3]Laboratoire Léon Brillouin, F-91191 Gif-sur-Yvette Cedex, France — [4]Jülich Centre for Neutron Science, D-85747 Garching, Germany — [5]Forschungsneutronenquelle Heinz Maier-Leibnitz, D-85747 Garching, Germany

Single crystals of $Ba_{1-x}Na_xFe_2As_2$ with $0.25 \leq x \leq 0.4$ have been studied by unpolarised and polarized neutron scattering. Unlike most FeAs-based compounds, Na doped $BaFe_2As_2$ exhibits two successive magnetic transitions at intermediate doping. First there is a transition into an antiferromagnetic phase with moments aligned along the plane, but at low temperatures spin reorient towards the *c* direction. The magnetic anisotropy of FeAs based compounds is thus of the easy plane type. In the range of coexisting antiferromagnetism and superconductivity we find very strong suppression of the ordered moments in the superconducting state. Inelastic experiments reveal a strong and sharp low-energy resonance in a sample with coexisting phases. This mode completely disappears upon increase of the doping and full suppression of the antiferromagnetic order.

TT 31.10 Tue 12:15 H 2053

Superconducting instabilities and quasipartical interference in the LiFeAs and Co-doped NaFeAs iron-based superconductors — •Dustin Altenfeld[1], Felix Ahn[1], Sergey Borisenko[2], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Leibniz-Institute for Solid State Research, IFW-Dresden, D-01171 Dresden, Germany

We analyze and compare the structure of the pairing interaction and superconducting gaps in LiFeAs and Co-doped NaFeAs by using the ten-orbital tight-binding model, derived from ab initio LDA calculations with hopping parameters extracted from the fit to ARPES experiments. We discuss the phase diagram and experimental probes to determine the structure of the superconducting gap in these systems with special emphasis on the quasiparticle interference, computed using the T-matrix approximation. In particular, we analyze how the superconducting state with opposite sign of the gaps on the two inner hole pockets in LiFeAs evolve upon changing the parameters towards NaFeAs compound.

TT 31.11 Tue 12:30 H 2053

Persistence of high-energy spin fluctuations in electron doped NaFeAs — •Jonathan Pelliciari[1], Yaobo Huang[1,2], Marcus Dantz[1], Valentina Bisogni[1], Paul Olalde Velasco[1], Changqing Jin[2], and Thorsten Schmitt[1] — [1]Paul Scherrer Institute, Villigen, Switzerland — [2]Institute of Physics Chinese Academy of Sciences, Beijing, China

Resonant Inelastic X-ray Scattering (RIXS) is a powerful method for probing spin fluctuations in cuprate and iron pnictide superconductors [1, 2]. We present a high resolution Fe L_3 RIXS study of parent and superconducting $NaFe_{1-x}Co_xAs$. Spectral shape decomposition reveals the persistence of broad dispersive magnetic excitations for all doping levels. In contrast to previous RIXS experiments on hole-doped $Ba_{1-x}K_xFe_2As_2$ compounds [1], the energy of such modes is not affected by doping. The magnetic weight per iron atom of such magnons and paramagnons remains constant. However, renormalized per formula unit the magnetic weight decreases with doping. We argue that cobalt-doping is mainly tuning the electronic correlations without affecting the dispersion range of the magnetic excitations, only reducing their intensity.

[1] K. J. Zhou et al, Nat. Comm., 4, 1470 (2013)
[2. M. P. M. Dean et al, Nature Materials 12, 1019 (2013)

TT 32: Transport: Topological Insulators 2 (jointly with DS, HL, MA, O)

Time: Tuesday 9:30–13:00 Location: H 3005

TT 32.1 Tue 9:30 H 3005

How electron-electron interactions may lead to a spontaneous time reversal symmetry breaking in (fractional) topological insulators — •Tobias Meng[1,2] and Eran Sela[3] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [3]Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Tel Aviv, 69978, Israel

We analyze the consequences of strong electron-electron interactions in topological insulators. Naively, topological insulators can be thought of as two copies of quantum Hall states for spin up and spin down electrons at opposite magnetic field, hence maintaining time reversal symmetry. Using an extension of the coupled-wire construction of quantum Hall states to systems with zero magnetic field, we find that interactions between electrons of spin up and spin down can stabilize a large family of fractional topological phases with broken time reversal invariance. The latter is manifest by a spontaneous spin polarization, a finite Hall conductivity, or by both. This suggests the possibility that strongly correlated fractional topological insulators may be unstable to spontaneous symmetry breaking.

TT 32.2 Tue 9:45 H 3005

Emergence of surface conductivity at low temperatures in FeSi — •Michael Wagner, Ralf Korntner, Andreas Bauer, and Christian Pfleiderer — Physik-Department, Technische Universität München, D-85748 Garching, Germany

We report a comprehensive study of the influence of the sample quality on the Hall-conductivity in the correlated semiconductor FeSi. For our study three high-quality $Fe_{1+x}Si$ single crystals with slightly different Fe concentrations x were grown by optical float zoning under ultra-high vacuum compatible conditions. While the magnetic properties vary sensitively for the samples studied, the transport properties display several key features that are independent of the Fe concentration. As our main result we find, that the Hall-conductivity of FeSi can be described in terms of a Drude-model. For low temperatures a second transport channel emerges besides bulk conductivity, which can be assigned unambiguously to the sample surface. Remarkably, the mobility of this surface conduction is extraordinarily high as compared to similar effects in conventional semiconductors, being quantitatively consistent with topological insulators such as Bi_2Te_3 where they are viewed as the signature of topologically protected transport channels.

TT 32.3 Tue 10:00 H 3005

Spin transport in 3d-topological insulator nanostructures — •Matthias Stosiek, Sven Essert, Cosimo Gorini, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

The spin-momentum locking for charge carriers on the surface of three-dimensional topological insulators holds promising prospects for spintronics applications. In this predominantly numerical study, we investigate the transport properties of nanostructures of 3d-TIs with ferromagnetic leads using model Hamiltonians. We also explore the influence of external electric and magnetic fields.

TT 32.4 Tue 10:15 H 3005

Tunnel Magnetoresistance scan of surface states of 3D topological insulators — •Sthitadhi Roy — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

The Fermi-surface of surface states of a 3D topological insulator (TI) has zero magnetization owing to time reversal symmetry, but an arbitrary segment of the full Fermi surface has a unique magnetic moment consistent with the type of spin-momentum locking. A three-terminal set up is proposed which directly couples to the magnetization of a chosen segment of a Fermi surface, hence leading to a finite tunnel magnetoresistance (TMR) response of the non-magnetic TI surface states, when coupled to spin polarized STM probe. This multi-terminal TMR reconstructs the in-plane momentum locked spin texture and also the out-of-plane spin polarization of hexagonally warped Fermi surfaces relevant for materials like Bi_2Te_3. This proposal is further extended to surfaces exposed by cleaving crystals at arbitrary angles to the crystal growth axis, and it shown that the TMR response not only probes and distinguishes these surfaces uniquely but the study of the spin textures for different surfaces put together acts like a hologram of the bulk band structure of the material.

TT 32.5 Tue 10:30 H 3005

Weak Antilocalization of 3DTI Surface States in the Presence of Spin-Orbit Impurities — •Pierre Adroguer[1], Weizhe Liu[2], Dimitrie Culcer[2] und Ewelina Hankiewicz[1] — [1]Institut füt Theoretische Physik und Astrophysik, Universität Würzburg, Deutschland — [2]School of Physics, The University of New South Wales, Sydney, Australia

The recent realization of three dimensional topological insulators (3DTIs) allows to probe the coherent transport of Dirac systems. In the presence of scalar disorder, weak antilocalization (WAL) is observed. However, TIs are materials where spin-orbit plays a crucial role, and the effect of spin-orbit impurities on coherent transport had not be studied yet.

In conventional electron gases where electrons have a parabolic dispersion, the concentration of spin-orbit impurities is of significative importance. Indeed, when the concentration of spin-orbit impurities is increased, the sign of the quantum correction to conductivity changes, going from weak localization to weak antilocalization (WAL).

In this work, we derive with the standard diagrammatic technique the quantum correction to conductivity when we add spin-orbit impurities to the diffusion of Dirac fermions in a disordered potential. We show that for every concentration of the spin-orbit impurities we

remain in the symplectic class of WAL. We also derive the value of this quantum correction to conductivity in the presence of a transverse magnetic field, and we show that fits with the conventional theory have to be revisited in the view of our results.

TT 32.6 Tue 10:45 H 3005

SmO thin films: a flexible route to correlated flat bands with nontrivial topology — •Deepa Kasinathan[1], Klaus Koepernik[2], Liu Hao Tjeng[1], and Maurits Haverkort[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Using density functional theory based calculations, we show that the correlated mixed-valent compound SmO is a 3D strongly topological semi-metal as a result of a $4f$-$5d$ band inversion at the X point. We also show that the topological non-triviality in SmO is very robust and prevails for a wide range of lattice parameters, making it an ideal candidate to investigate topological nontrivial correlated flat bands in thin-film form. Moreover, the electron filling is tunable by strain. In addition, we find conditions for which the inversion is of the $4f$-$6s$ type, making SmO to be a rather unique system. The similarities of the crystal symmetry and the lattice constant of SmO to the well studied ferromagnetic semiconductor EuO, makes SmO/EuO thin film interfaces an excellent contender towards realizing the quantum anomalous Hall effect in a strongly correlated electron system.

15 min. break.

Invited Talk TT 32.7 Tue 11:15 H 3005

Interacting Topological Insulators — •Stephan Rachel — Institut für Theoretische Physik, Technische Universität Dresden

The physics of electronic correlations in systems with topological band structures is a young and exciting field. In this talk, I will give an overview of the most relevant and interesting interaction effects in 2D and 3D topological insulators. Specifically, I will address the physics of the Kane-Mele-Hubbard model, the prototypical model of a correlated topological insulator, and its descendants in 2D as well as topological Mott insulators emerging in 3D topological band structures. Eventually, I will explain how strong interactions can affect the surface states of strong topological insulators and lead to even more exotic phases.

TT 32.8 Tue 11:45 H 3005

Interplay of topology and interactions in the quantum Hall regime of two-dimensional topological insulators — •Stefan Jürgens, Maxim Kharitonov, and Björn Trauzettel — Institute of Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

We study a class of two-dimensional topological insulators, in which the single-particle edge states are preserved in the presence of the magnetic field by a symmetry (e.g., crystalline) other than time-reversal. We focus on the vicinity of the crossing point between the zero-mode Landau levels. At half-filling, Coulomb interactions become particularly strong and lead to the formation of the quantum Hall "ferromagnetic" state with gapped charge excitations in the bulk. We identify the phases of this state that have gapped or gapless collective charge edge excitations and are characterized by the presence or absence of spontaneous symmetry breaking. The transitions between these phases can occur either continuously (via second order) or abruptly (via first order), depending on the parameters of the system. These transitions are accompanied by the corresponding behavior of the egde gap, which could be detected in transport measurements. Our findings provide an example of the interplay of topological and interaction-induced (spontaneous symmetry breaking) phenomena in the strong coupling regime.

TT 32.9 Tue 12:00 H 3005

Superconducting proximity effect in three-dimensional topological insulators in the presence of external magnetic fields — •Pablo Burset, Grigory Tkachov, Ewelina Hankiewicz, and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

The proximity induced pair potential in a topological insulator-superconductor hybrid features an interesting superposition of conventional spin-singlet potential from the superconductor and spin-triplet pairing induced by the surface state of the topological insulator. We theoretically describe ballistic junctions between superconductors and topological insulators under external magnetic fields. We use Green functions techniques to calculate experimentally relevant transport signatures like normal-superconductor tunnel spectroscopy, local density of states, and Josephson current. Additionally, we consider the effect of both topological order and an external magnetic field in the superconducting correlations. We associate the unconventional transport signatures with the symmetry of the singlet and triplet components of the pair potential.

TT 32.10 Tue 12:15 H 3005

Non-universal conductance fluctuations in 3D topological insulator nanowires. — •Emmanouil Xypakis[1], Jens H Bardarson[1], Louis Veyrat[2], Joseph Dufouleur[2], and Romain Giraud[2] — [1]Max-Planck-Institut fuer Physik Komplexer Systeme, Noethnitzer Straße 38, D-01187 Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research, IFW Dresden, D-01069 Dresden, Germany

The topic of this talk is a joint theoretical and experimental study of conductance fluctuations in 3D strong topological insulator nanowires. Specifically, when a nanowire is subjected to a magnetic field and disorder weak enough to be away from the universal diffusive limit, the amplitude of the conductance fluctuations oscillates with respect to the magnetic field along the wire. We explain this oscillatory behaviour by the Dirac nature of the topologically protected surface quasiparticles of the topological insulator. We further demonstrate the robustness of this quasi-ballistic transport regime by a direct comparison with experimental data obtained for Bi_2Se_3 nanowires.

TT 32.11 Tue 12:30 H 3005

How dephasing and charge puddles affect the edge transport in 2d-topological insulators — •Sven Essert, Viktor Krueckl, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

State of the art 2d-TI material systems show a length dependent non-quantized conductance for sample sizes larger than one micron. This feature is so far not well understood: Coherent elastic backscattering is symmetry forbidden and the observed weak temperature dependence does not seem to match the predictions for inelastic backscattering. We analytically and numerically investigate the effects of a third mechanism which was proposed to play a major role for the edge resistance: The combined effect of dephasing and elastic backscattering in charge puddles which are known to exist in the experimental samples.

We extract a range of dephasing times which are consistent with the experimental results. In addition, we make predictions for experiments on artificial charge puddles from which the real dephasing time scale could be determined.

TT 32.12 Tue 12:45 H 3005

Anderson localization at the edge of a 2D topological insulator — •Eslam Khalaf and Pavel Ostrovsky — Max Planck institute for solid state research, Stuttgart, Germany

We study transport via edge modes in a 2D topological insulator. Topological protection prevents complete localization of the edge states; however, quantum interference effects are still relevant for the transport properties at finite length scales. We mainly focus on the two most experimentally relevant cases: (i) a junction between two quantum Hall insulators with different filling factors and hence an imbalance in the number of right- and left-propagating modes (symmetry class A) and (ii) a relatively thick HgTe quantum well in the insulating state with an arbitrary number of edge modes (symmetry class AII). We derive the distribution of transmission probabilities as a function of the distance between leads. This allows us to demonstrate topological effects in the average conductance and the shot noise of the setup. We also consider mesoscopic fluctuations and compute the variance of conductance. This quantity is strongly influenced by topology in the quantum Hall case. All the calculations are carried out assuming localization effects are weak, i.e., in the short length limit. Technically, this amounts to studying 1D non-linear sigma model with a proper topological term and source fields on the semiclassical level. Remarkably, the semiclassical limit of the 1D sigma model can be exactly mapped onto a fully quantum 0D sigma model of a different symmetry class. This allows us to identify the distribution of transmission probabilities with the spectrum of a certain random matrix.

TT 33: Low-Dimensional Systems: Other Materials

Time: Tuesday 9:30–12:15 Location: H 3010

TT 33.1 Tue 9:30 H 3010

NMR on the Antiferromagnetic S=1/2 Heisenberg Spin Chain Sr_2CuO_3 under the Impact of Ni Impurities — •Yannic Utz[1], Franziska Hammerath[1], Satoshi Nishimoto[1], Stefan-Ludwig Drechsler[1], Neela Sekhar Beesetty[2], Romuald Saint-Martin[2], Alexandre Revcolevschi[2], Christian Hess[1], Bernd Büchner[1], and Hans-Joachim Grafe[1] — [1]IFW Dresden, Germany — [2]SP2M-ICMMO UMR-CNRS, Université Paris-Sud, France

We present ^{63}Cu NMR measurements on single crystals of Sr_2CuO_3 doped with different amounts of nickel and compare them to numerical DMRG results. The parent compound contains copper-oxygen chains with S=1/2 on the copper site coupled by a large antiferromagnetic exchange coupling $J \approx 2000$ K and is known to be a good realization of the 1D Heisenberg model. The measurements show that replacing only a few of the S=1/2 Cu ions with S=1 Ni has a major impact on the magnetic properties of the spin chain system. An unusual line broadening in the low temperature NMR spectra reveals the existence of an impurity-induced local alternating magnetization (LAM), and exponentially decaying spin-lattice relaxation rates T_1^{-1} towards low temperatures indicate the opening of a spin gap similar to Ca-doped Sr_2CuO_3 [1]. While the T_1^{-1} measurements could be explained by pure chain segmentation, as expected for a S=0 impurity, the spectra can only be understood by taking the nickel.

[1] F. Hammerath et al., Phys. Rev. B 89, 184410 (2014).

TT 33.2 Tue 9:45 H 3010

Thermodynamic investigations of the quasi-2d triangular Heisenberg antiferromagnet $Cs_2CuCl_2Br_2$ — •Ulrich Tutsch, Lars Postulka, Bernd Wolf, Michael Lang, Natalija van Well, Franz Ritter, Cornelius Krellner, and Wolf Assmus — Physikalisches Institut, Goethe-University Frankfurt (M), SFB/TR 49

The system $Cs_2CuCl_{4-x}Br_x$ ($0 \leq x \leq 4$) is a quasi-two-dimensional Heisenberg antiferromagnet with a triangular in-plane arrangement of the spin-spin couplings. The ratio J'/J of the corresponding coupling constants determines the degree of frustration in the system and has been found to be 0.34 ($x = 0$) and 0.74 ($x = 4$) [1] for the border compounds. One may ask whether for some intermediate Br concentration an even higher degree of frustration can be reached. Indeed, some indications have been reported by Ono *et al.* [1]. Here, we present specific heat C and susceptibility χ measurements below 1 K in magnetic fields B up to 13.5 T for the intermediate compound $Cs_2CuCl_2Br_2$, which, due to site-selective substitution, shows a well-ordered halide sublattice. Indications for an antiferromagnetic transition are observed around 90 mK for $B = 0$. A small field of $B = 0.14$ T is sufficient to fully suppress this anomaly. Taking into account the high saturation field of about 20 T, extrapolated from $\chi(T = \text{const}, B)$ scans at low temperatures, this small ordered region in the B-T plane clearly indicates a high degree of frustration in $Cs_2CuCl_2Br_2$.

[1] T. Ono *et al.*, J. Phys. Soc. Jpn. **74** (2005) Suppl. pp. 135-144.

TT 33.3 Tue 10:00 H 3010

Weakly coupled spin-dimer systems based on stable organic biradicals — •Bernd Wolf[1], Lars Postulka[1], Ulrich Tutsch[1], Martin Baumgarten[2], Yulia Borozdina[2] und Michael Lang[1] — [1]Physics Institute, Goethe-University Frankfurt (M), SFB/TR 49, D-60438 Frankfurt (M), Germany — [2]Max-Planck-Institute for Polymer Research, SFB/TR 49, D-55128 Mainz, Germany

We present low-temperature susceptibility data of newly synthesized $S = 1/2$ spin-dimer systems consisting of stable organic biradicals, formed by bridging nitronyl-nitroxides (NN) and imono-nitroxides (IN) via tolane molecules. The choice of this bridging molecule ensures a moderately strong intra-dimer coupling constant J_{intra}/k_B around 9.0 K (NN) and 4.3 K (IN). In addition, a weak coupling between the spin dimers of the order of 1 K can be inferred from high-temperature susceptibility data. The crystal structure suggests a 2D arrangement of the dimer units. To determine potential field-induced ordered phases, highest-resolution AC-susceptibility measurements have been performed down to a temperature of $T = 27$ mK and magnetic fields up to $B = 10.5$ T. We observed for both materials double-peak structures in the susceptibility below the saturation field. For a detailed understanding, especially with regard to the dimensionality of the magnetic interactions and the nature of the field-induced magnetic order, we compare the experimental results with measurements on metal-organic coupled dimer compound $C_{36}H_{48}Cu_2F_6N_8O_{12}S_2$, which shows clear signatures of 2D physics [1].

[1] Tutsch et al., Nat. Commun. 5, 5169 (2014).

TT 33.4 Tue 10:15 H 3010

Low-energy effective interactions beyond cRPA by the functional renormalization group — •Michael Kinza and Carsten Honerkamp — Institutit für theoretische Festkörperphysik, RWTH Aachen University

In the derivation of low-energy effective models for solids targeting the bands near the Fermi level, the constrained random phase approximation (cRPA) has become an appreciated tool to compute the effective interactions. Here we present applications of a constrained functional renormalization group (cfRG) scheme to two simple multi-band systems and compare the resulting effective interactions to the cRPA. The employed wick-ordered fRG scheme generalizes the cRPA approach by including all interaction channels in an unbiased way. First we consider a multiband model for graphene, where we integrate out the σ-bands to get an effective theory for π-bands. It turns out that terms beyond cRPA are strongly suppressed by xy-plane reflection-symmetry of the bands and that in our model, the cRPA stays qualitatively correct even if one breaks this symmetry slightly. The second example is a model for a Cu-O-chain, where we consider an effective theory for the Cu 3d-orbital. Here the fRG data points to relevant corrections compared to the cRPA results.

15 min. break.

TT 33.5 Tue 10:45 H 3010

Ultrafast optical spectroscopy of quasi one dimensional Ta_2NiSe_5 — •Selene Mor, Marc Herzog, Claude Monney, Julia Stähler, and Martin Wolf — Fritz-Haber-Institut der MPG, Dep. of Phys. Chem., Berlin, Germany

Ta2NiSe5 is a layered compound in which atomic chains are aligned in the layers, forming a quasi one dimensional crystal structure. At 328 K, the system shows a structural change, which is accompanied by an electronic phase transition from a semiconductor to an excitonic insulator, with an estimated energy gap of about few hundreds millielectronvolts. Our aim is to unveil the microscopic mechanisms underlying the phase transition in Ta_2NiSe_5. The system is excited with a femtosecond Ti:sapphire fundamental laser pulse and the mid-infrared (MIR) transient optical response is monitored by ultrafast optical spectroscopy. We observe a fast rise of transient reflectivity, which decays exponentially. This incoherent response is superimposed by a coherent phonon oscillation. A preliminary study with white light (WL) probe beam shows that low repetition rate is mandatory to study the response of the photoexcited system. The analysis unveils the presence of two phonons at 3 and 4 THz, that dominate at high (HT) and low (LT) temperature, respectively. We study the time evolution of the two phonons in the LT phase. We reveal a finite lifetime for the LT phase phonon, whose amplitude decays within few picoseconds, while the HT phase phonon amplitude remains almost constant. The picture is supported by temperature-dependent Raman spectroscopy.

TT 33.6 Tue 11:00 H 3010

Structural effects on charge order in single-layered manganites $R_{1-x}A_{1+x}MnO_4$ — •Johannes Engelmayer, Holger Ulbrich, Lisa Weber, Markus Braden, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Germany

Single-layered manganites show a complex interplay between charge, orbital, and magnetic degrees of freedom. For half-doped ($x = 1/2$) $R_{1-x}A_{1+x}MnO_4$ ($R = \text{Pr, La}$; $A = \text{Ca, Sr}$) the so-called Goodenough model is well established. This model proposes a site-centered charge order with a checkerboard pattern of Mn^{3+} and Mn^{4+} ions accompanied by an orbital order. Furthermore a magnetic order develops with ferromagnetic three-spin zig-zag chains and antiferromagnetic interchain coupling. For $x = 2/3$ the charge order appears as stripe pattern with two adjacent stripes of Mn^{4+} ions alternating with a single stripe of Mn^{3+} ions, while in the magnetically ordered state four-spin zigzag chains arise [1]. For a deeper understanding of the emergence of

charge order, it is appropriate to vary on the one hand the elements R and A while keeping the doping level x constant—involving structural changes at fixed charge carrier density—and on the other hand change the doping level with the same R and A. Therefore various single crystals of $R_{1-x}A_{1+x}MnO_4$ with R = (Pr, Nd, Sm, Tb), A = (Ca, Sr) and $0.5 \leq x \leq 0.7$ were grown and their structural parameters were determined by x-ray diffraction. Based on measurements of resistivity, magnetization, specific heat, and crystal structure we discuss the influence of structural variations on the ordering temperature.

[1] H. Ulbrich, M. Braden, Physica C **481**, 31 (2012)

TT 33.7 Tue 11:15 H 3010

Effect of Cu Doping on the Phonon Softening in $TiSe_2$ — •Roland Hott, Rolf Heid, and Frank Weber — Karlsruhe Institute of Technology, Institute of Solid State Physics, P.O.B. 3640, D-76021 Karlsruhe, Germany

We investigated the effect of Cu doping on the soft-mode behaviour of phonons in the Charge Density Wave (CDW) system $TiSe_2$ both experimentally by means of high resolution Inelastic X-ray Scattering (IXS) and theoretically in Density Functional Theory (DFT) based ab-initio phonon calculations. Within this theoretical framework the experimentally observed hardening of the soft phonons can not be explained in terms of a simple charge doping effect but it is due to a substantial change of the ionic displacement forces due to the additional Cu ion potentials.

[1] F. Weber et al., Phys. Rev. Lett. 107 (2011) 266401.

TT 33.8 Tue 11:30 H 3010

Electron Energy-Loss Spectroscopy on the Dichalcogenide 2H-MoS_2 — •Carsten Habenicht, Martin Knupfer, and Bernd Büchner — Institute for Solid State Research, IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Two-dimensional transition metal dichalcogenides may complement graphene in future applications. This requires a detailed knowledge of their electronic properties. We have investigated the electronic excitations in 2H-MoS_2 using electron energy-loss spectroscopy (EELS). The electron energy-loss spectra of 2H-MoS_2 in the (100) and (110) directions were measured for various momentum transfer values. The results allow the identification of the A and B exciton peaks and, in particular, their energy-momentum dispersion. The dispersions exhibit approximately quadratic upward trends and slight anisotropies in the (100) and (110) directions. The dispersions allow the estimation of the effective masses of the excitons which are in close proximity to predicted values.

TT 33.9 Tue 11:45 H 3010

Doping dependence of the plasmon dispersion in 2H-$TaSe_2$ and related systems — •Eric Müller, Carsten Habenicht, Martin Knupfer, and Bernd Büchner — IFW-Dresden, P.O.Box 270116, DE-01171 Dresden, Germany

The electronic excitations of 2H-$TaSe_2$ and related single crystalline systems have been investigated using electron energy-loss spectroscopy. These systems consist of hexagonal layers with weak interlayer van-der-Waals bonding. We show the influence of alkali metal intercalation on the energy position and the dispersion of the charge-carrier plasmon. Further we demonstrate how the slope of dispersion is affected by the additional charge and the change of charge-carrier density in consequence. Our results indicate a universal evolution of the plasmon dispersion independent of the intercalant (Na, K) and the dichalcogenide ($TaSe_2$, TaS_2, $NbSe_2$).

TT 33.10 Tue 12:00 H 3010

ARPES and NMTO Wannier Orbital Theory of $Li_{0.9}Mo_6O_{17}$ — •L. Dudy[1], J.W. Allen[2], J.D. Denlinger[3], J. He[4], M. Greenblatt[5], M.W. Haverkort[6], O.K. Andersen[7], and Y. Nohara[7] — [1]Physikalisches Institut, Universität Würzburg, D- 97074 Würzburg, Germany — [2]University of Michigan, Ann Arbor, MI, USA — [3]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [4]Clemson University, Clemson, SC, USA — [5]Rutgers University, Piscataway, NJ, USA — [6]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [7]Max-Planck-Institut für Festkörperphysik, Stuttgart, Germany

$Li_{0.9}Mo_6O_{17}$ displays theoretically interesting [1] metallic quasi-one dimensional (1D) behavior that is unusually robust against 3D crossover with decreasing temperature, and is characterized by a large value of anomalous exponent $\alpha \approx 0.6$ [2]. We present very high resolution, low temperature (T=6K-30K) angle resolved photoemission spectroscopy (ARPES) of its band structure and Fermi surface (FS), analyzed with N-th order muffin tin orbital (NMTO) Wannier function band theory. We confirm a previous conclusion [3] that LDA band theory is unusually successful, implying a small Hubbard U, and find in ARPES the dispersion and FS warping and splitting expected for predicted small and long range hoppings ($t_\perp \approx$ 10-15 meV) between chains.

[1] P. Chudzinski, T. Jarlborg and T. Giamarchi, Phys. Rev. B 86, 075147 (2013).
[2] L. Dudy et al., J. Phys. Cond. Matter 25, 014007 (2013).
[3] M. Nuss and M. Aichhorn, Phys. Rev. B 89, 045125 (2014).

TT 34: Transport: Graphene (jointly with CPP, DS, DY, HL, MA, O)

Time: Tuesday 9:30–12:15 Location: A 053

TT 34.1 Tue 9:30 A 053

Observation of supercurrent in graphene-based Josephson junction — •Libin Wang[1], Chuan Xu[2], Sen Li[1], Wencai Ren[2], and Ning Kang[1] — [1]Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing 100871, China — [2]Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China

Josephon junctions with a normal metal region sandwiched between two superconductors (S) are known as superconductor- normal-superconductor (SNS) structures. It has attracted significant attention especially when changing the normal metal with graphene, which allow for high tunability with the gate voltage and to study the proximity effect of the massless Dirac fermions. Here we report our work on graphene-based Josephon junction with a new two dimensional superconductor crystal, which grown directly on graphene, as superconducting electrodes. At low temperature, we observer proximity effect induced supercurrent flowing through the junction. The temperature and the magnetic field dependences of the critical current characteristics of the junction are also studied. The critical current exhibits a Fraunhofer-type diffraction pattern against magnetic field. Our experiments provided a new route of fabrication of graphene-based Josephon junction.

TT 34.2 Tue 9:45 A 053

Magnetoresistance of nanocrystalline and ion-irradiated graphene — •Paul Linsmaier[1], Lorenz Weiss[1], Armin Shaukat[1], Christian Bäuml[1], Daniel Steininger[1], Ina Schneider[1], Matthias Büenfeld[2], Nils-Eike Weber[2], Andrey Turchanin[2], Miriam Grothe[3], Thomas Weimann[3], Ferdinand Kisslinger[4], Heiko B. Weber[4], and Christoph Strunk[1] — [1]Inst. f. Exp. and Appl. Physics, University of Regensburg — [2]Fac. of Physics, University of Bielefeld — [3]Physikalisch-Technische Bundesanstalt, Braunschweig — [4]Fac. of Physics, F.-A. University Erlangen-Nürnberg

We investigate the magnetotransport in Hall bar structures of nanocrystalline graphene [1] compared to Ar^+-bombarded epitaxial graphene [2]. We measured the resistance $R(T)$ and $R(B)$ for samples with different sheet resistance (10-40 kΩ/sq at T = 300K). The I-V characteristics of both types show strong non-linear behavior at low temperatures. Low resistive samples of nanocrystalline graphene show positive magnetoresistance (MR) with values up to + 60 % in perpendicular magnetic field for temperatures below a crossover temperature. Above this temperature the MR becomes negative. The perpendicular MR in the ion-bombarded graphene was always negative. In parallel magnetic field the MR exhibits large positive values up to + 700 % in the nanocrystalline graphene. Strongly non-monotonic behavior of the MR was observed in the ion-bombarded sample in parallel field.

[1] A. Turchanin et al., ACS Nano 5 (2011).
[2] K. V. Emtsev et al., Nat. Mat. 8, 203 - 207 (2009).

TT 34.3 Tue 10:00 A 053

Aharonov-Bohm effect in a graphene ring encapsulated in hexagonal boron nitride — •Jan Dauber[1,2], Martin Oellers[1], Alexander Epping[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], Fabian Hassler[4], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Jülich, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan — [4]JARA-Institute for Quantum Information at RWTH Aachen University, Aachen, Germany

Recent developments in the van der Waals assembly of heterostructures of two-dimensional materials enable the fabrication of graphene on substrate with very high quality. Outstanding charge carrier mobility and mean free path have been reported for micrometer sized samples of graphene encapsulated in hexagonal boron nitride (hBN). These unique electronic properties offer opportunities for the observation of rich mesoscopic transport phenomena in sub-micron sized graphene-hBN devices. Here, we present low-temperature magnetotransport measurements on a high mobility graphene ring encapsulated in hexagonal boron nitride. We observe the co-existence of weak localization, Aharonov-Bohm (AB) oscillations and universal conductance fluctuations. We investigate the periodicity of the AB oscillations as a function of charge carrier density and find clear evidence of the AB effect even at very low carrier densities. Finally, we report on the investigation of the AB oscillations in the cross over regime of emerging quantum Hall effect at reasonable magnetic fields.

TT 34.4 Tue 10:15 A 053

Ab-initio simulations of local current flows in functionalized graphene flakes and ribbons — •Michael Walz[1], Jan Wilhelm[2], Alexei Bagrets[1], and Ferdinand Evers[3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [2]Institute of Physical Chemistry, University of Zürich, CH-8057 Zürich, Switzerland — [3]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

Using our DFT-based transport framework AITRANSS [1], we calculate the transmission and the local current density in graphene flakes functionalized by adsorbed atoms, such as nitrogen or hydrogen. We find that even a single nitrogen atom can almost completely suppress the conductance of a (gated) graphene armchair nano-ribbon. In this situation local ring currents emerge that result in local (orbital) magnetic moments.

In addition, the current flow shows a highly inhomogeneous structure. In the absence of any scatters, the current flows along parallel streamlines that exhibit a strong lateral modulation [2]. In the presence of scattering centers, such as 20% hydrogen absorbants, we observe a filamentary pattern of streamlines. It exhibits local ring currents ("eddies") that go along with sizeable local magnetic fields, $\mathbf{B}(\mathbf{r})$. [3]

In the future, we plan to study the statistics of local currents of such large flakes and its dependency on the impurity concentration.

[1] A. Arnold, F. Weigend, F. Evers, J. Chem. Phys. 126 (2007)
[2] J. Wilhelm, M. Walz, F. Evers, Phys. Rev. B 89 (2014)
[3] M. Walz, J. Wilhelm, F. Evers, Phys. Rev. Lett. 113 (2014)

TT 34.5 Tue 10:30 A 053

Fabry-Pérot interference in monolayer and bilayer graphene devices — •Ming-Hao Liu and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

Recent progress on high-quality graphene device fabrications has made submicron- or even micron-scale phase-coherent phenomena in graphene experimentally observable. Hence reliable quantum transport simulations for ballistic graphene devices are nowadays highly demanded. In this talk we give an overview on how such simulations can be accurately and efficiently performed. Concrete examples of Fabry-Pérot interference in single pn junctions in suspended monolayer graphene [1], multiple pn junctions in monolayer graphene on substrate [2], and pnp junctions in bilayer graphene encapsulated by hexagonal boron nitrite [3] will be briefly shown, as well as further studies of "electron optics" in graphene.

[1] P. Rickhaus, R. Maurand, M.-H. Liu, M. Weiss, K. Richter, and C. Schönenberger, Nature Comm. **4**, 2342 (2013); M.-H. Liu, et. al., arXiv:1407.5620 (2014).
[2] M. Drienovsky, F.-X. Schrettenbrunner, A. Sandner, D. Weiss, J. Eroms, M.-H. Liu, F. Tkatschenko, and K. Richter, Phys. Rev. B **89**, 115421 (2014).
[3] A. Varlet, M.-H. Liu, V. Krueckl, D. Bischoff, P. Simonet, K. Watanabe, T. Taniguchi, K. Richter, K. Ensslin, and T. Ihn, Phys. Rev. Lett. **113**, 116601 (2014).

TT 34.6 Tue 10:45 A 053

Substrate-Induced doping of supported graphene: an ab initio study — •Arezoo Dianat[1], Rafael Gutierrez[1], Zhongquan Liao[2], Martin Gall[2], Ehrenfried Zschech[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Fraunhofer Institute for Ceramic Technologies and Systems, D-01109 Dresden, Germany

A major challenge for applications of graphene in nanoelectronics is the absence of a band gap in its low energy spectrum. One possibility of gap opening is doping and there are various methods to achieve it: evaporation, thermal treatment, and plasma doping. In this study, using ab initio molecular dynamics, we investigate graphene doping mediated by substrate-induced mechanisms. More specifically, we address graphene on a B-doped Si(100) surface. Our ab initio total energy calculations show that B atoms prefer to locate on the surface layer of Si(100). Further, intercalation of B atoms into vacancy positions of graphene is only found for temperatures larger than 700 K. In a second step, the electrical transport properties of B-doped graphene are studied using the non-equilibrium Green's function approach.

15 min. break.

TT 34.7 Tue 11:15 A 053

Density of states of graphene with vacancies — •Soumya Bera — MPI-PKS, Dresden

We numerically calculate the density of states (DOS) of graphene in the presence of compensated vacancy disorder. The model belongs to the BDI class of Atland-Zirnbauer symmetry classification of disordered metals, where the non-linear Sigma model predicts a Gade-type singularity in the DOS $\rho(E) \sim E^{-1}\exp(-|\log(E)|^{-1/2})$. We show that in the pre-asymptotic regime this is indeed true, however, at even lower energies the Gade-type behavior gives away to a stronger singularity of the form $\rho(E) \sim E^{-1}|\log(E)|^{-x}$ with $2 > x \geq 1$ in agreement with recent analytical work (Ostrovsky et al., PRL 113, 186803). We conclude that the generic Sigma model of the BDI class does not apply for strong (unitary) scatterers; the nature of disorder is of important to determine the low energy behaviour of disordered graphene.

[1] PRL 113, 186802 (2014).

TT 34.8 Tue 11:30 A 053

Nonlocal optical excitations and dynamic shear viscosity of graphene — •Julia Link, Peter P. Orth, and Jörg Schmalian — Institute for Theoretical Condensed Matter physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe

We study the dynamic shear viscosity of the interacting electronic fluid of graphene in the finite frequency, collision-less regime, relevant for nonlocal optical properties. We determine the frequency dependence of the dynamic shear viscosity for non-interacting graphene and study the influence of the long-range Coulomb interaction. Finally we discuss a setup where the viscosity can be spectroscopically measured.

TT 34.9 Tue 11:45 A 053

Transport phenomena in deformed graphene: Magnetic field versus curvature — Thomas Stegmann[1,2] and •Nikodem Szpak[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany — [2]Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca, Mexico

The current flow in deformed graphene nanoribbons is studied theoretically. Using a tight-binding model, we apply the nonequilibrium Green's function (NEGF) method to investigate how a localized deformation and a perpendicular magnetic field affect the current flow. At long wavelengths, the eikonal approximation applied to the effective Dirac equation leads to the Mathisson-Papapetrou equations describing trajectories of a spinning point-like particle in a curved space. We show that these trajectories are compatible with the current flow paths of the NEGF calculations. The deformation has two-fold effect on them: First, via a pseudo-magnetic field, with sixfold symmetry of attractive and repulsive regions, which acts differently on electrons and holes, but changes its sign when going from the K to the K' point. Second, via an attractive force due to the curvature of the ribbon, which treats electrons and holes equivalently. We conclude with an outlook on how to use deformed graphene ribbons for geometrical focusing of

the current flow.

TT 34.10 Tue 12:00 A 053

Merging of the Dirac points in electronic artificial graphene — •Juraj Feilhauer[1,2], Walter Apel[1], and Ludwig Schweitzer[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany — [2]Institute of Electrical Engineering, Slovak Academy of Sciences, Bratislava, Slovakia

Artificial graphene (AG) is a man-made electron system which has a similar bandstructure as normal graphene, i.e. in the low-energy part of the electronic spectrum, two bands touch and form a pair of Dirac cones. We study analytically and numerically the bandstructure of electronic AG under uniaxial strain. Here, AG is created from the two-dimensional electron gas by applying a repulsive triangular potential and the effect of strain is modeled by tuning the distance between the repulsive potentials along the armchair direction. In normal graphene, the theory based on nearest-neighbour tight-binding approximation predicts that due to the change of the hopping integrals by applying uniaxial strain, both Dirac cones are shifted away from the corners of the Brillouin zone and also becomes elliptical instead of circular. With increasing compressive strain, the Dirac cones move along the edge of Brillouin zone towards each other until they merge. We show that such a merging of the Dirac cones also exists in uniaxially compressed AG. With applied strain, we find the Dirac cones are also tilted and that can be simulated by the presence of a next-nearest-neighbour hopping in the tight-binding hamiltonian. We discuss a possible realization of our theoretical results in a recent experiment with molecular graphene.

TT 35: PhD Symposium: Quantum Phase Transitions: Emergent Phenomena beyond Elementary Excitations (organized by MA, jDPG)

Organizers: G. Benka, P. Geselbracht, F. Rucker, S. Säubert, and C. Schnarr (TU München)

Traditionally, physics has focused on understanding the stable phases of matter like superconductivity or magnetism. Particle like states, dominating the low-energy physics of such systems, so-called elementary excitations, have been studied extensively in the past century and play an important role in our understanding of solid state physics. Modern material science and new experimental techniques, however, led to the discovery of completely different types of states, in which all electronic properties are dominated by a continuum of fluctuations. Such states arise in the vicinity of phase transitions, which are accessed by the variation of a non-thermal control parameter at zero temperature, so-called quantum phase transitions. Even though quantum phase transitions are strictly defined to be at zero temperature, the quantum critical continuum which surrounds continuous quantum phase transitions can influence electronic systems over a wide range of the phase diagram. This leads to the emergence of unique properties, new phenomena as unconventional superconductivity and the breakdown of the concept of elementary excitations. While the research on quantum phase transitions has started in a small community with the investigation of materials with strong electronic correlations, the interest in this field of research has grown fundamentally in the past years. This is attributed to the discovery of materials, which are much easier to access experimentally, as well as to the fact that the theoretical concepts are relevant to a broad range of physics. This makes quantum phase transitions one of the most vivid research topics in physics over the past decade. This symposium brings together the most recognized international speakers of this field to give a tutorial introduction to conventional and unconventional quantum criticality as well as to highlight recent experimental and theoretical advances. The interplay between tutorials and up to date research talks addresses a very broad audience and will stimulate an interdisciplinary exchange of knowledge which makes this field of research attractive for a larger community. Quantum phase transitions represent a very important area of research for a broad community of PhD students with rather different background. Keeping up to date with such an active field of research, however, is very demanding and time consuming for PhD students, as appropriate further training possibilities are only rarely offered and often focus on extremely specialised topics. This symposium will offer such an opportunity for PhD students working on quantum phase transitions, as well as for students and physicists working in other areas.

Time: Tuesday 9:30–16:30 Location: EB 301

Invited Talk TT 35.1 Tue 9:30 EB 301

Experimental Studies of Quantum Phase Transitions — •Andrew Mackenzie — Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

In my lecture I will review what is known about quantum criticality produced by tuning systems close to magnetic instabilities. I will discuss the key physics behind quantum criticality, and then describe some model experimental systems. I will concentrate on the importance of thermodynamic measurements in classifying both quantum criticality and the novel phases that form in its vicinity.

Invited Talk TT 35.2 Tue 10:15 EB 301

Metallic Quantum Ferromagnets — •Manuel Brando — Max Planck Institute for Chemical Physics of Solids, Noethnitzer Str. 40, 01187 Dresden, Germany

In my talk I will review studies on quantum criticality with focus on metallic ferromagnets. The existence of a ferromagnetic quantum critical point has been a matter of discussion as long as 40 years ago, but had been dismissed in the past 15. During the last years several ferromagnetic metals have been tuned across the ferromagnetic quantum phase transition. Here, astonishing discoveries were made that are extending our understanding of ferromagnetic quantum criticality.

TT 35.3 Tue 10:45 EB 301

Neutron-Depolarisation Imaging of the Ferromagnetic Quantum Phase Transition in ZrZn2 — •Philipp Schmakat[1,2], Marco Halder[1], Georg Brandl[1,2], Michael Schulz[2], Stephen Hayden[3], Robert Georgii[2], Peter Böni[1], and Christian Pfleiderer[1] — [1]Physik Department E21, Technische Universität München, Germany — [2]Forschungs-Neutronenquelle Heinz Maier-Leibnitz, D-85748 Garching, Germany — [3]H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, United Kingdom

When a polarised neutron beam traverses a ferromagnetic material, the orientation and strength of the polarisation changes sensitively as a function of the ferromagnetic moment and the size of the ferromagnetic domains. We have developed an experimental set up that allows

to perform neutron depolarisation imaging as a function of magnetic field. In a study of the ferromagnetic quantum phase transition in the weak itinerant ferromagnet ZrZn2 under pressure we find, that a peculiar field dependence of the neutron depolarisation survives on the paramagnetic side of the temperature versus pressure phase diagram. This provides putative evidence for the emergence of complex magnetic textures.

30 min. Coffee Break

Invited Talk TT 35.4 Tue 11:30 EB 301

Theoretical Concepts of Quantum Phase Transitions — •Matthias Vojta — Technische Universität Dresden, Germany

This tutorial will cover theoretical concepts and ideas for the description of quantum phase transitions. Starting from order parameters and order-parameter field theories, it will discuss critical exponents and scale invariance, the fascinating interplay of classical and quantum mechanical fluctuations at finite temperatures, and the quantum-to-classical correspondence. Further topics will include interaction-driven metal-insulator transitions, topological phase transitions, and the role of quenched disorder. Throughout the talk, microscopic models will be used for illustration.

Invited Talk TT 35.5 Tue 12:15 EB 301

Quantum criticality and beyond — •Andrew Schofield — School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham, B15 2TT United Kingdom.

The exploration of quantum critical points has provided an extraordinarliy fruitful direction for experimentalists and theorists alike to investigate new ordering principles for correlated matter. Beyond the basic concepts, the field has a number of outstanding questions which motivate current research - from the interplay between critical fluctuations and other forms of order, to the theoretical framework which governs quantum critical behaviour in physical systems. My talk will explore these questions and their context.

TT 35.6 Tue 12:45 EB 301

Universal Postquench Prethermalization at a Quantum Critical Point — •Pia Gagel[1], Peter Orth[1], and Jörg Schmalian[1,2] — [1]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Institute for Solid State Physics, Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany

We consider an open system near a quantum critical point that is suddenly moved towards the critical point. The bath-dominated diffusive nonequilibrium dynamics after the quench is shown to follow scaling behavior, governed by a critical exponent that emerges in addition to the known equilibrium critical exponents. We determine this exponent and show that it describes universal prethermalized coarsening dynamics of the order parameter in an intermediate time regime. Implications of this quantum critical prethermalization are: (i) a power law rise of order and correlations after an initial collapse of the equilibrium state and (ii) a crossover to thermalization that occurs arbitrarily late for sufficiently shallow quenches.

Lunch Break

Invited Talk TT 35.7 Tue 14:00 EB 301

Quantum Criticality in Quantum Magnets — •Christian Rüegg — Paul Scherrer Institute, Laboratory for Neutron Scattering and Imaging, Switzerland — University of Geneva, Department of Quantum Matter Physics, Switzerland

Quantum magnets are exceptional solid-state model systems for high-precision studies of quantum criticality [1]. Recent results from such studies include complex phases like spin Luttinger-liquids and excitations realized in low-dimensional and frustrated systems [2-4], the exciting physics of impurities and quenched disorder [5], and fractionalization and the emergence of novel excitations near quantum critical points [2,6]. Studies of model oxides and halides by neutron scattering and complementary experimental techniques will be presented. These experimental results will be discussed in the context of recent developments of powerful computational methods enabling fully quantitative analysis and of related work on other model systems like gases of ultracold atoms.

[1] T. Giamarchi et al., Nature Physics 4, 198 (2008). [2] B. Thielemann et al., Phys. Rev. Lett. 102, 107204 (2009). [3] Y. Kohama et al., Phys. Rev. Lett. 109, 167204 (2012). [4] F. Casola et al., Phys. Rev. Lett. 110, 187201 (2013). [5] S. Ward et al., J. Phys.: Condens. Matter 25, 014004 (2013). [6] P. Merchant et al., Nature Physics 10, 373 (2014).

TT 35.8 Tue 14:30 EB 301

Spin Hall effect in two-dimensional systems — •Annika Johansson[1], Christian Herschbach[1,2], Dmitry Fedorov[2,1], and Ingrid Mertig[1,2] — [1]Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

A relativistic phase shift model (RPSM), derived as a generalization of the resonant scattering model [1-4], was introduced recently [5] to describe the skew-scattering mechanism of the spin Hall effect (SHE) caused by impurities in bulk crystals. The RPSM was found to be an appropriate model to obtain a simple qualitative description of the SHE for dilute bulk alloys based on host crystals with free-electron like Fermi surfaces and weak spin-orbit coupling [6].

Here, we present its analogue for two-dimensional (2D) systems. The proposed 2D-RPSM provides good qualitative agreement with *ab initio* results obtained for dilute alloys based on one-monolayer noble metal films. However, the colossal SHE caused by Bi impurities [7] is not reproduced due to a strong influence of vertex corrections for these systems not properly taken into account by the model. The relation of the 2D-RPSM to the 2D resonant scattering model [8] is also discussed.

[1] A. Fert *et al.*, J. Magn. Magn. Mater. **24**, 231 (1981); [2] G.Y. Guo *et al.*, PRL **102**, 036401 (2009); [3] A. Fert and P.M. Levy, PRL **106**, 157208 (2011); [4] P.M. Levy *et al.*, PRB **88**, 214432 (2013); [5] D.V. Fedorov *et al.*, PRB **88**, 085116 (2013); [6] A. Johansson *et al.*, J. Phys.: Condens. Matter **26**, 274207 (2014); [7] C. Herschbach *et al.*, PRB **90**, 180406(R) (2014); [8] B. Gu *et al.*, arXiv:1402.3012.

Invited Talk TT 35.9 Tue 14:45 EB 301

Beyond quantum phase transitions — •Wilhelm Zwerger — TU Muenchen

The talk will discuss quantum phase transitions in the context of ultra cold gases in optical lattices. Moreover, it will address the issue of quantum phase transitions which show up only in dynamical properties, the so called many-body localization.

TT 35.10 Tue 15:15 EB 301

Topological superconductivity and unconventional pairing in oxide interfaces — •Mathias Scheurer[1] and Jörg Schmalian[1,2] — [1]Institut für Theorie der kondensierten Materie (Karlsruher Institut für Technologie), Karlsruhe, Deutschland — [2]Institut für Festkörperphysik (Karlsruher Institut für Technologie), Karlsruhe, Deutschland

To pinpoint the microscopic mechanism for superconductivity has proven to be one of the most outstanding challenges in the physics of correlated quantum matter. Thus far, the most direct evidence for an electronic pairing mechanism is the observation of a new symmetry of the order parameter, as done in the cuprate high-temperature superconductors. Alternatively, global, topological invariants allow for a sharp discrimination between states of matter that cannot be transformed into each other adiabatically. In this talk we present an unconventional pairing state for the electron fluid in two-dimensional oxide interfaces and establish a direct link to the emergence of nontrivial topological invariants. Topological signatures, in particular Majorana edge states, can then be used to detect the microscopic origin of superconductivity. In addition, we show that the density wave states that compete with superconductivity have very rich spatial textures (magnetic vortices, Skyrmions) and sensitively depend on the nature of the pairing interaction.

TT 35.11 Tue 15:30 EB 301

Quantum criticality in frustrated $CePd_{1-x}Ni_xAl$ — •Akito Sakai[1], Stefan Lucas[2], Veronika Fritsch[1,3], Philipp Gegenwart[1], Oliver Stockert[2], and Hilbert v. Löhneysen[3] — [1]Universität Augsburg, Institut für Physik, Elektronische Korrelationen und Magnetismus, Germany — [2]Max-Planck-Institut für chemische Physik fester Stoffe, Dresden, Germany — [3]Karlsruher Institut für Technologie, Physikalisches Institut, Germany

Various interesting behaviors such as non-Fermi liquid and unconventional superconductivity have been observed in the vicinity of quantum critical points (QCPs), which are induced by the competition between Kondo effect and RKKY interaction. Another route to achieve the QCP is geometric frustration. CePdAl is one of the candidates of such

quantum critical frustrated systems [1, 2]. In addition to the heavy fermion behaviors, a partial antiferromagnetic ordering is revealed below $T_N = 2.7$ K, where one third of the Ce moments in the distorted kagomé lattice are still paramagnetic [1]. In this presentation, we discuss the possible QCP in $CePd_{1-x}Ni_xAl$ revealed by the specific heat measurement in the dilution refrigerator.

[1] A. Dönni *et al.*, J. Phys.: Condens. Matter **8**, 11213 (1996).
[2] V. Fritsch *et al.*, Phys. Rev. B **89**, 054416 (2014).

TT 35.12 Tue 15:45 EB 301

Resonant inelastic x-ray scattering of magnetic excitations in the novel 5d^4 iridate Ba_2YIrO_6 — •Maximilian Kusch[1,2], T. Dey[1], A. Maljuk[1], S. Wurmehl[1], B. Büchner[1,2], V. M. Katakuri[3], B. H. Kim[3], D. V. Efremov[3], J. van den Brink[3], M. Moretti[4], M. Krisch[4], and J. Geck[1] — [1]Institute for Solid State and Materials Research, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Institut für Festkörperphysik, Technische Universität D-01062 Dresden, Germany — [3]Institute for Theoretical Solid State State Physics, IFW Dresden, Germany — [4]ESRF, B.P.220, 38043 Grenoble, France

In contrast to the much studied 5d^5 iridates with a spin-orbit coupled J=1/2 ground state, Ba_2YIrO_6 is a realization of a Ir-5d^4 system. For this case, a ground state J=0 is expected, i.e, Ba_2YIrO_6 should be non-magnetic. Surprisingly, our measurements of the magnetic susceptibility reveal sizable magnetic moments whose microscopic origin is still unclear. Theoretical studies indicate the important role of low-lying magnetic excitations, thereby providing a possible explanation for the unexpected magnetic susceptibility [Khaliullin Phys. Rev. Lett. 111 (2013)]. In addition, our theoretical models predict a considerable dispersion of the J=1 and J=2 excitations in Ba_2YIrO_6. To elucidate the unconventional magnetism of Ba_2YIrO_6 and to determine the dispersions of the J=1 and J=2 excitations experimentally, we performed RIXS studies of this novel 5d^4 compound. Here we present the results, focusing on the magnetic dispersions in a large region of q-space in comparison to our model calculations.

Posters

TT 35.13 Tue 16:15 EB 301

Fermi surface on the border of Mott transition in NiS_2 — •Hui Chang[1], Sven Friedemann[1,2], Monika Gamza[3], William Coniglio[4], David Graf[4], Stan Tozer[4], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]HH Wills Laboratory, University of Bristol, UK — [3]Department of Physics, Royal Holloway, University of London, Egham, UK — [4]National High Magnetic Field Laboratory, Tallahassee, Florida 32310, USA

The transition from a metallic to a correlated, or Mott, insulating state is a long-standing theme of fundamental interest in condensed matter research. Using quantum oscillation measurements in high magnetic fields to probe the electronic Fermi surface and effective carrier mass on the metallic side of the transition could provide much needed microscopic information. In the cuprates, such studies in samples doped into the metallic state have identified the Fermi surface structure in underdoped and overdoped regimes. Because the quantum oscillation signal is strongly suppressed in the presence of disorder, pressure rather than doping should ideally be used to reach the metallic state. We present the first observation of quantum oscillations from a pressure-metallised 3D Mott insulator. NiS_2 can be tuned through the Mott transition at a modest pressure of 30kbar. Quantum oscillations near the Mott transition are observed with the tunnel diode oscillator technique in magnetic fields up to 31T. The main observed oscillation frequency is consistent with the Fermi surface obtained within density functional theory, whereas the effective mass is significantly enhanced over the band mass.

TT 35.14 Tue 16:15 EB 301

Transport properties across the quantum phase transitions in $Mn_{1-x}Fe_xSi$ — •Fabian Jerzembeck[1], Marlies Gangl[1], Anna Kusmartseva[1,2], Andreas Bauer[1], and Christian Pfleiderer[1] — [1]Physik Department, Technische Universität München, D-85747 Garching, Germany — [2]Department of Physics, Loughborough University, UK-LE11 3TU Leicestershire, United Kingdom

Recent theory identify the thermal and electrical transport properties as a sensitive probe of the validity of the Fermi liquid description of the metallic state [1]. A prime example for a well understood, weakly spin-polarized Fermi liquid ground state has long been established in the weak itinerant helimagnet MnSi. We report a detailed study of the evolution of the thermal and electrical transport properties across the quantum phase transitions in $Mn_{1-x}Fe_xSi$ [2] down to temperatures of ∼2 K under magnetic fields up to 14 T. These data are complemented by additional selected measurements in $Mn_{1-x}Co_xSi$. As our main objective we consider the validity of the Wiedemann-Franz law across the quantum phase transitions in $Mn_{1-x}Fe_xSi$.

[1] R. Mahajan, M. Berkeshli, S. A. Hartnoll, Phys. Rev. B **88**, 125107 (2013). [2] A. Bauer *et al.*, Phys. Rev. B **82**, 064404 (2010).

TT 35.15 Tue 16:15 EB 301

Identification of a Brazovskii quantum phase transition in the Chiral Magnet MnSi — •Jonas Kindervater[1], Stefan Ernst[1], Andreas Bauer[1], Wolfgang Häussler[1,2], Nicolas Martin[1,2,3], Peter Böni[1], Markus Garst[4], and Christian Pfleiderer[1] — [1]Physik-Department, Technische Universität München, Germany — [2]Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany — [3]CEA Saclay, DSM/IRAMIS/Laboratoire Leon Brillouin, France — [4]Institute for Theoretical Physics, Universität zu Köln, Germany

In the chiral magnet MnSi the transition into the ordered phase is driven to first-order due to strongly interacting fluctuations, which can be explained within the framework of the Brazovskii scenario [1]. We report a small angle neutron scattering and high resolution neutron spin echo spectroscopy study on the quantum phase transition in $Mn_{1-x}Fe_xSi$. Upon suppressing the helimagnetic order by iron doping a putative quantum phase transitions is observed [2]. According to theory [3], a possible Brazovskii quantum phase transition might thereby be realized either as a first- or second-order transition or, alternatively, as a tricritical point. Our study gives insight in the precise nature of the strongly interacting chiral fluctuations and the nature of the quantum phase transitions realized in $Mn_{1-x}Fe_xSi$.

[1] M. Janoschek *et al.*, PRB **87**, 134407 (2013); [2] A. Bauer *et al.*, PRB **82**, 064404 (2010); [3] J. Schmalian and M. Turlakov, PRL **93**, 036405 (2004)

TT 35.16 Tue 16:15 EB 301

Tuning $ZrFe_4Si_2$ by Ge substitution: confirming the proximity to a magnetic quantum critical point — •Katharina Weber[1,2], Nandang Mufti[1], Til Goltz[2], Theo Woike[3], Hans-Henning Klauss[2], Christoph Bergmann[1], Helge Rosner[1], and Christoph Geibel[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Institute of Solid State Physics, TU Dresden, Germany — [3]Institute for Structural Physics, TU Dresden, Germany

Magnetic systems with reduced dimensionality or frustration are attracting strong interest because these features lead to an increase of quantum fluctuations which often results in unusual, very interesting properties. Our previous studies evidence the AFe_4X_2 family (A = Y, Lu, Zr and X = Ge, Si) to cover the whole regime from frustrated antiferromagnetic (AFM) order up to the quantum critical point (QCP) separating the frustrated AFM ground state from the paramagnetic ground state. $ZrFe_4Si_2$ showed evidence for an unusual type of weak magnetic order and was therefore suspected to be near the QCP. In order to get a deeper insight into its ground state, we performed a detailed study of Ge substituted $ZrFe_4Si_2$, where Ge is suspected to stabilize the magnetic state because of a negative chemical pressure effect. We synthesized polycrystalline samples of $ZrFe_4(Si_{1-x}Ge_x)_2$ with $x = 2\,\%$ to $50\,\%$ and investigated their magnetic, thermodynamic, structural and transport properties. As expected with increasing Ge content the magnetic state is stabilized towards a well defined AFM order at high Ge content. This confirms the near-by QCP in $ZrFe_4Si_2$.

TT 36: Organic Electronics and Photovoltaics: Transport of Charges – from Molecules to Devices (jointly with CPP, HL)

Time: Tuesday 9:30–13:00 Location: C 130

TT 36.1 Tue 9:30 C 130

Electronic properties of biphenylene and the biphenylene carbon sheet — •Johann Lüder, Biplab Sanyal, Olle Eriksson, Carla Puglia, and Barbara Brena — Department of Physics and Astronomy, Uppsala University, Sweden

Biphenylene ($C_{12}H_8$) is a promising candidate for applications in molecular electronics as well as a building block for two dimensional materials such as the biphenylene carbon (BPC) sheet, a possible alternative for graphene in nanoelectronics. The electronic structure of the gas phase biphenylene molecule is measured by core and valence level spectroscopy and detailed insights are revealed in conjunction with Density Functional Theory calculations. Hybrid functional calculations including the recently proposed OT-RSH functional are compared to GW calculations to provide an accurate theoretical description. Using the band structure obtained from GW calculations, we compute the optical adsorption spectrum by solving the Bethe-Salpeter equation of BPC. Typically for two-dimensional materials, a strong excitonic effect is found and bright and dark excitons are determined.

TT 36.2 Tue 9:45 C 130

Dimensionality of excitation transport in sol-gel-derived polymeric carbon nitride photocatalysts — •Christoph Merschjann[1,2], Stefanie Tschierlei[1], Kamalakannan Kailasam[3], Arne Thomas[3], Dirk Hollmann[4], and Stefan Lochbrunner[1] — [1]Institut für Physik, Universität Rostock, D-18051 Rostock, Germany — [2]Freie Universität Berlin, D-14195 Berlin, Germany — [3]Leibniz-Institut für Katalyse, D-18059 Rostock, Germany — [4]Technische Universität Berlin, D-10623 Berlin, Germany

The spectral and temporal development of optically excited states in highly active sol-gel-derived polymeric carbon nitride (SG-CN) photocatalysts is investigated using time-resolved optical spectroscopy. By combining transient absorption results from a femtosecond pump-probe setup and transient photoluminescence using streak-camera investigations, the evolution of a light-emitting species appearing upon UV excitation is obtained. The emission decay reveals a universal power-law behaviour over more than seven decades in time (150 fs to 5 μs), the main difference between samples being the characteristic decay time in the nanosecond range. This finding is consistently described using a random-walk approach for the diffusive transport of light-induced polaron pairs, including both geminate and bimolecular recombination mechanisms. Thus, important features of the light-induced charge transport, namely the dimensionality and the regime of reasonable carrier mobilities, are deduced.

The validity of the approach is shown via comparison to ESR-based carrier-density measurements and photocatalytic activities.

TT 36.3 Tue 10:00 C 130

Simulation of Charge Transport in Organic Self-Assembled Monolayers for Applications in Field-Effect Transistors — •Susanne Leitherer[1], Christof Jäger[2], Marcus Halik[3], Tim Clark[2], and Michael Thoss[1] — [1]Institute for Theoretical Physics, University Erlangen-Nürnberg, Germany — [2]Computer-Chemie-Centrum, University Erlangen-Nürnberg, Germany — [3]Institute of Polymer Materials, University Erlangen-Nürnberg, Germany

We study charge transport through self-assembled monolayers (SAMs), which are used in field-effect transistors [1], employing a combination of molecular-dynamics simulations, semiempirical electronic structure calculations and Landauer transport theory. In particular, we investigate SAMs consisting of multifunctional molecules, where the active π-system is linked to a flexible insulating alkyl-chain. We find a close relation between the transport characteristics and the structural and electronic properties of the SAM [2]. For selected systems, we analyze pathways for efficient charge transport by examining local currents in the molecular layers. The pathways are compared to those obtained using Metropolis Monte Carlo (MC) path searches. In order to study the time-dependence of the preferred electron paths, we consider snapshots of the system selected at different times of a MD simulation. To further examine the influence of fluctuations on the transport properties, we utilize a time-dependent approach of charge transport using time-dependent nonequilibrium Green's function (NEGF) theory.

[1] C. Jäger *et al.*, J. Am. Chem. Soc. **135**, 4893 (2013)
[2] S. Leitherer *et al.*, J. Chem Phys. **140**, 204702 (2014)

TT 36.4 Tue 10:15 C 130

Quantum Molecular Dynamics Studies of Polymer-based Thermoelectric Materials — •Håkan W. Hugosson, Amina Mirsakiyeva, and Anna Delin — Department of Materials och Nano Physics, Royal Institute of Technology KTH, Stockholm, Sweden

Using modern quantum molecular dynamics methods (QMD), where all the interactions are calculated from an electronic structure method (here density functional theory - DFT), we study the polymer-based thermoelectric material PEDOT and its charge carrying polarons. QMD simulations are parameter-free and enable a direct and potentially unbiased simulation of chemical and physical events. Since temperature is taken into account a sampling of the conformational space is made, also making simulations less biased upon choices of e.g. initial conditions and chosen reaction coordinates. Among these studies we will focus on the theoretical modeling of the properties and dynamics of polarons and bipolarons in PEDOT-oligomers and crystals and the effect of novel dopants in PEDOT.

Organic polymer-based thermoelectric materials (like PEDOT), unlike presently used inorganic thermoelectric materials composed of hazardous elements with low natural abundance, though presently being less efficient, can be mass-produced at a low cost using safer abundant elements.

TT 36.5 Tue 10:30 C 130

First-principles based descriptor for intrinsic charge carrier mobility in organic devices — •Christoph Schober, Karsten Reuter, and Harald Oberhofer — Technische Universität München

In organic electronics charge carrier mobility is a key performance parameter. Due to the complex manufacturing processes of e.g. organic field effect transistors (OFETs) measured mobilities are often heavily affected by the device preparation. This masks the intrinsic materials properties and therewith hampers the decision whether further device optimization for a given organic molecule is worthwhile or not. Within hopping models based e.g. on Marcus theory the intrinsic mobility can be reliably calculated from first principles. Using a perturbative approach to this theory we formulate a descriptor that can be efficiently calculated for a wide range of organic molecules. For this descriptor we obtain good correlations to fully calculated mobilities, as well as to highest-quality experimental data where device preparation uncertainties are minimized. This suggests the descriptor as a useful tool for materials screening and quick assessment of device-related influences in measured mobilities.

TT 36.6 Tue 10:45 C 130

Effect of Mesoscale Ordering on the Energy Landscape of a Conjugated Polymer — •Carl Poelking, Patrick Gemünden, Kurt Kremer, Kostas Daoulas, and Denis Andrienko — Max Planck Institute for Polymer Research, Mainz, Germany

A multiscale simulation approach is proposed to study the effect of morphology on charge transport properties of polymeric semiconductors, with poly(3-hexylthiophene) as a test case. The method incorporates both long-range conformational disorder and local ordering, and permits reintroduction of atomistic details into large-scale morphologies generated with a coarse-grained simulation approach. Based on the resulting atomistically resolved mesophases, we investigate how the energy landscape and spatial correlations thereof evolve with increasing degree of structural order in partially ordered systems. We show that a shift towards larger conjugation lengths plays a role in the amplification rather than formation of low-energy states, such that decreased energetic disorder rather than a decreased energetic mean characterize energetics in crystalline domains.

TT 36.7 Tue 11:00 C 130

The role of microstructure on charge transport in semicrystalline polymers — •Riccardo Di Pietro[1], Iyad Nasrallah[2], Joshua Carpenter[3], Lisa Koelln[4], Lars Thomsen[5], Christopher R. McNeill[6], Antonio Facchetti[7], Harald W. Ade[3], Hen-

ning Sirringhaus[2], and Dieter Neher[4] — [1]Hitachi Cambridge Laboratory, UK — [2]University of Cambridge, UK — [3]North Carolina State University, Raleigh, USA — [4]University of Potsdam, Germany — [5]Australian Synchrotron, Clayton, Australia — [6]Monash University, Clayton, Australia — [7]Polyera Corporation, Skokie, USA

We present a study on charge transport on two widely used semiconducting polymers, P(NDI2OD-T2) and P3HT. Combining field effect transistor characterization and charge accumulation spectroscopy we provide a consistent and unambiguous correlation between the charge density dependence of mobility and the semicrystalline morphology of the polymer film. This new experimental evidence demonstrates that charge transport in semicrystalline polymers cannot be described using any currently available charge transport model such as multiple trap and release or variable range hopping. A new charge transport model is therefore proposed, which explicitly accounts for the presence of both crystalline and amorphous regions within the polymer film and for the coulobic repulsion between charge carriers accumulated within the same crystallite. It finally provides a coherent picture of charge transport that has important general consequences in regimes that are relevant not only for transistors but also diodes and solar cells.

15 min. break.

TT 36.8 Tue 11:30 C 130

The molecular structure of a high electron mobility n-type copolymer [P(NDI2OD-T2)] as studied by Infrared Transition Moment Orientational Analysis [IR-TMOA] — •Arthur Markus Anton[1], Robert Steyrleuthner[2], Wilhelm Kossack[1], Dieter Neher[3], and Friedrich Kremer[1] — [1]Institut für Experimentelle Physik I, Universität Leipzig, Germany — [2]Fachberich Physik, Freie Universität Berlin, Germany — [3]Institut für Physik und Astronomie, Universität Potsdam, Germany

To investigate the molecular order in thin layers of P(NDI2OD-T2) a novel technique, named Infrared Transition Moment Orientational Analysis (IR-TMOA), is employed. Structure-specific vibrational bands are analyzed in dependence on *polarization and inclination* of the sample film with respect to the optical axis. Making use of IR specificity we deduce the molecular order parameter tensor for the respective moieties with regard to the sample coordinate system and determine separately the orientation of atomistic planes defined through the naphthalenediimide (NDI) and bithiophene (T2) units relative to the substrate, and hence, relative to each other. We observe that chlorobenzene causes the T2 planes to align preferentially parallel to the substrate at an angle of 29°. A chloronaphthalene:xylene mixture, instead, gives rise to a reorientation of the T2 units from a *face on* into an *edge on* arrangement (65 to 70°). In contrast, the NDI part remains basically unaffected. For both solvents, evidence for aggregated chains is observed by UV/vis absorption spectroscopy [Steyrleuthner et al., *J. Am. Chem. Soc.* **136** (2014)].

TT 36.9 Tue 11:45 C 130

Aerosol Jet-Printed Organic Thin Film Transistors - Performance Analysis and Optimization — •Arno John, Hanna Krikcziokat, and Klaus Meerholz — Institut für Physikalische Chemie, Universität Köln

For the success of organic thin film transistors (OTFTs) in industrial applications it is essential to process devices by printing in order to radically lower production costs. Aerosol jet is a direct-write printing method which provides the user great control over material deposition. Along with layout flexibility and material compatibility, this makes this printing technology an excellent tool for fast prototyping devices.

We use aerosol jet technology to fabricate entire p- and n-type OTFTs by printing Ag-ink (source/drain electrodes), PTAA (p-type semiconductor) and N2200 (n-type semiconductor), PMMA (dielectric) and PEDOT:PSS (gate electrode). By varying parameters for individual components and evaluating the resulting transistors we optimize the printing process.

The performance of printed components is compared to evaporated and spin coated transistor components. We show that, with optimized processing parameters, it is possible to print transistors with charge carrier mobility, output current on/off ratio and threshold voltage of nearly equal quality of non-printed transistors.

TT 36.10 Tue 12:00 C 130

Investigation of semiconducting polymers with thermally cleavable side chains for application in multilayer devices I: Morphology and OFET devices. — •Janusz Schinke[1,2], Sabina Hillebrandt[2,3], Milan Alt[2,5], Torben Adermann[2,4], Tobias Glaser[2,3], Annemarie Pucci[2,3], Norman Mechau[2,5], Manuel Hamburger[2,4], Wolfgang Kowalsky[1,2], and Robert Lovrincic[1,2] — [1]TU Braunschweig, IHF, Germany — [2]InnovationLab GmbH, Heidelberg, Germany — [3]U. Heidelberg, KIP, Germany — [4]U. Heidelberg, OCI, Germany — [5]KIT, Germany

Conjugated polymers enable the production of electronic devices from solution at room temperature due to their advantageous combination of their electrical, optical and film-forming properties. A major milestone for this emerging technology consists in achieving printed multi-layer functional devices. A great challenge for printed organic electronics is to deposit the subsequent layer of a multilayer component from the same solvent without destroying the underlying freshly deposited layer. The solubility reduction of semiconducting molecules by the external stimulus of heat is the aim of our work. Novel organic semiconductors bearing thermally cleavable side chains were investigated via AFM, ellipsometry, PE spectroscopy and IR spectroscopy. Their charge transport characteristics were studied using OFETs. These methods allow us to obtain a clear understanding of the pyrolysis process and its influence on the resulting performance. We achieve very homogeneous layers after thermal treatment which exhibit excellent solvent resistance and additionally show an increase in OFET performance.

TT 36.11 Tue 12:15 C 130

Following the evolution of nanomorphology in PEDOT:PSS electrodes in-situ — •Claudia Palumbiny[1], Feng Liu[2], Thomas P. Russell[2], Alexander Hexemer[3], Cheng Wang[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]University of Massachusetts Amherst, Department of Polymer Science and Engineering, 120 Governors Drive, Amherst, MA 01003, USA — [3]Lawrence Berkeley National Lab, Advanced Light Source, 1 Cyclotron Road, Berkeley, CA 94720, USA

The strongest advantages of organic photovoltaics over classical semiconductors are the possibility of fully flexible devices and easy upscaling, e.g. by slot-die printing. For fully printed and flexible devices there is a strong need for non-brittle and solvent processed electrodes, such as highly conductive PEDOT:PSS. Film properties are strongly correlated to the films nanomorphology and with this strongly depend on the processing technique used. We investigate the film evolution of highly conductive PEDOT:PSS in-situ during the printing process. We monitor the film evolution by in-situ grazing incident wide angle scattering (GIWAXS). Five film formation processes are detected, the crystallization of the polymers is correlated to solvent evaporation and enhanced interchain coupling is induced by the use of high boiling point co-solvents as ethylene glycol. The enhanced conductivity in co-solvent treated PEDOT:PSS films is related to enhanced interchain coupling, change of the PEDOT to PSS ratio and crystallite sizes.

[1] Palumbiny et al., J. Phys. Chem. C 2014, 118, 13598.

TT 36.12 Tue 12:30 C 130

Angle resolved spectroscopy resolving local morphology of organic optoelectronic materials — •Marius van den Berg, Anke Horneber, Kathrin Swider, Martin Meixner, and Dai Zhang — 1Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany

The main component on which organic photovoltaic, transistor and photodetectors rely is the optoelectronic material. Knowledge about the local photophysical and photochemical properties of these materials at nanometer scale is important for improving overall performance and applicability [1]. The crystallinity and domain size of the local donor/acceptor morphology strongly affect the photon-electron conversion efficiencies of organic photovoltaics [2,3]. We aim at understanding the influences of nanometer scale morphology on the photophysical processes between donors and acceptors using a home built parabolic mirror assisted microscope. Using polarized excitation spectroscopy and angle resolved photoluminescence spectroscopy, we determine the relative degree of local structural order and molecular orientation in intact and photo degraded optoelectronic polymers. Furthermore, intensity changes in the angle resolved photoluminescence signals are compared with changes in the local photocurrent, to investigate morphology related photo degradation procedures, as well as the reversible/irreversible degradation steps in pi-conjugated polymers. 1)A. Dupuis et al. Eur. Phys. J. Appl. Phys. 56, 34104 (2011) 2)X. Wanget al. Small, 7, 2793 (2011) 3)R. Noriega et al. Nat. Mater., 12, 1038-1044, (2013)

TT 36.13 Tue 12:45 C 130

Multifunctional SNOM and its Application in Imaging Optoelectric Materials — Anke Horneber, Marius van den Berg, Martin Meixner, Kathrin Swider, and •Dai Zhang — Institute of Physical and Theoretical Chemistry, University of Tübingen

Optoelectronic polymer material is the basic component in photovoltaic, photodetector, or transistor system. In organic photovoltaic, the photon-electron conversion efficiency is strongly influenced by the local donor/acceptor morphology, such as crystalline, or domain size.

To get insight into this topic, we developed multifunctional scanning near-field microscopy allowing simultaneously collecting correlated topographical, optical (Raman scattering and fluorescence), and photocurrent signals with nanometer scale resolutions [1-3]. The distributions and local morphology of donor or acceptor materials are imaged using the Raman fingerprints and scanning probe microscopes. The intensity ratios between the donor photoluminescence and the local photocurrent will be discussed, with respect to the charge transfer processes in films of different morphologies. Furthermore, photodegradation will be compared, especially in the aspects of local morphology, and optical properties. References: [1] Zhang, D. et al, Phys. Rev. Lett., 2010, 104, 056601. [2] Wang, X., Azimi, H., Zhang, D., et al, Small, 2011, 7, 2793. [3] Wang, X., Egelhaaf, H., Zhang, D., Adv. En. Mater, 2014, 1400497. [4] Wang, X., Broch K., Zhang, D. et al., J. Phys. Chem. Lett., 2014, 5, 1048.

TT 37: Thermoelectric Materials (organized by DS)

Time: Tuesday 9:30–11:00 Location: H 0111

TT 37.1 Tue 9:30 H 0111

Complete thermoelectric material characterization at high temperatures — •Hendrik Kolb[1], Titas Dasgupta[2], Johannes de Boor[1], Knud Zabrocki[1], and Eckhard Müller[1,3] — [1]Institute of Materials Research, German Aerospace Center — [2]Dept. of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay — [3]Institute of Inorganic and Analytical Chemistry, Justus-Liebig-Universität Gießen

Thermoelectricity is the direct conversion of thermal energy into electrical energy and can be used for the recovery of waste heat into electrical power. For an efficient research process a quick characterization is crucial to see the effects of the material manufacturing process on the thermoelectric properties. The three thermoelectric key quantities can strongly be temperature dependent, which makes a complete characterization over a wide temperature range necessary. The special feature of our system is the additional direct zT measurement by the Harman method independently from the single measurements to verify the results. The better comparability of the measured properties is one main advantage in a simultaneous measurement, because all quantities are measured at one temperature step. Additionally the measurement uncertainty which can easily reach more than 20% in the zT measurement due to methodical or geometrical differences in different setups is reduced. We show results for a complete high temperature characterization of thermoelectric materials up to 650 K and show good agreement with reference data. Also, we demonstrate the influence of radiation losses on thermal conductivity measurement.

TT 37.2 Tue 9:45 H 0111

Enhanced transport properties of rutile oxides — •Denis Music and Jochen M. Schneider — Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany

Oxide based thermoelectrics offer potential for high efficiency thermoelectric conversion for harvesting electricity from heat, but suffer from a low power factor due to the low electrical conductivity. We used quantum mechanical calculations to identify alloying elements for RuO2 with enhanced Seebeck coefficient. We probed all 3d and 4d transition metals as well as all lanthanides and identified Fe and La to be the most promising candidates as a manifold increase in Seebeck coefficient was predicted. This materials design proposal was then critically evaluated by measuring the Seebeck coefficient of sputter-deposited thin films. Furthermore, the electrical and thermal conductivity was measured. Saturated RuO2 with Fe and La exhibit not only a fourfold increase in the Seebeck coefficient, but also a decrease in thermal conductivity. This yields the highest power factor reported for RuO2 despite a twofold decrease in the electrical conductivity. Hence, the ab initio predictions regarding the Seebeck coefficient are validated by experiments. Furthermore, Fe and La lead to grain refinement and a more porous morphology. Our results suggest that maximizing the structural distortion of RuO2 by dilute alloying with selected transition metals and lanthanides can increase the Seebeck coefficient and decrease the thermal conductivity by fostering quantum confinement and phonon scattering, respectively. Other rutile oxides, such as MnO2, will also be discussed.

TT 37.3 Tue 10:00 H 0111

Reduced thermal conductivity of TiNiSn/HfNiSn superlattices — •Paulina Holuj[1,3], Christoph Euler[1], Tino Jaeger[1], Benjamin Balke[2], and Gerhard Jakob[1,3] — [1]Institute of Physics, University of Mainz, Staudinger Weg 9, 55128, Germany — [2]Institute of Inorganic and Analytical Chemistry, University of Mainz, Staudinger Weg 9, 55128, Germany — [3]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128, Germany

Thermoelectric materials possess the ability to convert unused heat to electricity. The efficiency of their operation depends on the dimensionless figure of merit $ZT = \frac{S^2\sigma}{\kappa}$ that contains only material dependent parameters (S - Seebeck coefficient, σ - electrical conductivity, κ - thermal conductivity). The goal of our work is to reduce thermal conductivity and doing so we aim to enhance ZT. Reduction of κ is achieved by scattering of phonons at interfaces of superlattices (SL) made out of TiNiSn and HfNiSn half-Heusler materials. Based on x-ray diffraction we assume to have sharp interfaces between constituent layers. In the current study we observe a systematic reduction of the thermal conductivity as the period of the SLs is decreasing with a clear minimum at about 3 nm and a further increase of κ due to formation of an artificial crystal.

We gratefully acknowledge financial support by DFG (Ja821/4-2) and the Graduate School of Excellence Material Science in Mainz (GSC 266).

TT 37.4 Tue 10:15 H 0111

Nanostructured SiGe thin films obtained through MIC processing — •Marc Lindorf[1], Hartmut Rohrmann[2], and Manfred Albrecht[1] — [1]University of Augsburg, Universitätsstraße 1, 86159 Augsburg, Germany — [2]Oerlikon Advanced Technologies AG, Iramali 18, 9496 Balzers, Liechtenstein

In times of growing energy consumption thermoelectric devices pose an opportunity for energy harvesting. However commercially available thermoelectric materials show a deficit in efficiency governed by low ZT values. New approaches like nanostructuring [1] try to increase the efficiency, but often lack industrial applicability due to high cost and low production speed. This work presents results on sputter deposited multilayer stacks of $Si_{80}Ge_{20}(10\,nm)/[Al(d_{Al})/Si_{80}Ge_{20}(10\,nm)]_{50}/SiO_2(200\,nm)/Si$. Crystallization and Al dopant activation is achieved by post-annealing through metal induced crystallization (MIC) [2]. This approach allows grain size control via annealing temperature and Al interlayer thickness d_{Al} in the nanometer regime. Results will be presented regarding structural and thermoelectric properties.

[1] Y. Lan et al.,*Adv. Funct. Mater.* **20**, 357-376 (2010).
[2] Z. M. Wang et al.,*Phys. Rev. Lett.* **100**, 125503 (2008)

TT 37.5 Tue 10:30 H 0111

The Influence of a Distinct Diameter Variation on the Thermal Conductivity of Individual Bismuth Telluride Nanowires — •Danny Kojda[1], Rüdiger Mitdank[1], Anna Mogilatenko[2], William Töllner[3], Zhi Wang[4], Michael Kröner[4], Peter Woias[4], Kornelius Nielsch[3], and Saskia F. Fischer[1] — [1]AG Neue Materialien, Humboldt-Universität zu Berlin, D-10099 Berlin — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, D-12489 Berlin — [3]Institut für Angewandte Physik, Universität Hamburg, D-20355 Hamburg — [4]Laboratory for Design of Microsystems, University of Freiburg - IMTEK, D-79110 Freiburg

Calculations on indented nanowires (NWs) have shown that surface morphology can affect the thermal conductivity λ by phonon backscat-

tering [1]. In order to determine the role of a distinct diameter variation, two $Bi_{0.39}Te_{0.61}$ NWs from the same batch are investigated by means of a combined full-thermoelectrical, structural and chemical characterization. Both NWs have the same chemical composition and the same direction of growth along the [110] direction. The NWs differ in their morphology. One NW shows a strong diameter variation between 190 nm and 320 nm and the other has a diameter of 187 nm with smooth sidewalls. At room temperature λ was determined by the 3ω-method and a reduction in the indented NW by about 50 % with respect to the smooth NW was observed. Hence, NW-vacuum interfaces perpendicularly arranged to the direction of transport can lead to a reduced λ in NWs [2]. [1] A. Moore *et al.*, 2008 APL, **93** 083112. [2] D. Kojda *et al.*, 2014 Semicond. Sci. Technol., **29** 124006.

TT 37.6 Tue 10:45 H 0111

Enhanced thermoelectric efficiency of *p*-type Half-Heuslers by intrinsic phase separation and carrier concentration optimization. — •Elisabeth Rausch[1,2], Claudia Felser[2], and Benjamin Balke[1] — [1]Institut für Anorganische und Analytische Chemie, Johannes Gutenberg-Universität, Mainz, Germany — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

State of the art *p*-type Half-Heusler compounds (space group $F\bar{4}3m$) for thermoelectric applications are found in the $MCoSb_{0.8}Sn_{0.2}$ (M = Ti/Zr/Hf) system. The outstanding properties are achieved by a nanostructuring approach via ball milling followed by a rapid consolidation method. We, herein report on a alternative approach to reduce the thermal conductivity, which is by an intrinsic phase separation. A optimum ratio of Ti to Hf in combination with an adjustment of carrier concentration via Sn substitution lead to a record thermoelectric figure of merit $ZT = 1.15$ for $Ti_{0.25}Hf_{0.75}CoSb_{0.85}Sn_{0.15}$. Our study is complemented by a long-term stability test under thermal cycling conditions in the interesting temperature range for automotive applications.

TT 38: Frontiers of Electronic Structure Theory: Nuclear Dynamics, Methods (jointly with O, HL)

Time: Tuesday 10:30–13:30 Location: MA 004

Invited Talk TT 38.1 Tue 10:30 MA 004

Electronic structure in the vicinity of strong non-adiabatic couplings — •Eberhard K.U. Gross — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The Born-Oppenheimer (BO) approximation is among the most fundamental ingredients of modern Condensed-Matter Theroy. Yet, some of the most fascinating phenomena such as the process of vision or phonon-driven superconductivity occur in the regime where the BO approximation breaks down. To tackle such situations one has to face the Hamiltonian of the complete system of interacting electrons and nuclei. We deduce an exact factorization [1] of the full electron-nuclear wavefunction into a purely nuclear part and a many-electron wavefunction which parametrically depends on the nuclear configuration. The resulting equations of motion for the nuclear and electronic wavefunctions lead to a unique definition of exact potential energy surfaces as well as exact geometric phases. We show an example [2] where the geometric phase associated with the conical intersection of BO surfaces has no counterpart in the true electron-nuclear wavefunction. In the time-domain, whenever there is a splitting of the nuclear wavepacket in the vicinity of an avoided crossing, the exact time-dependent surface shows a nearly discontinuous step [3], reminiscent of Tully surface hopping algorithms. Based on this observation we propose novel mixed-quantum-classical algorithms.

[1] Abedi, Maitra, Gross, PRL 105, 123002 (2010).
[2] Min, Abedi, Kim, Gross, PRL 113, 263004 (2014).
[3] Abedi, Agostini,Suzuki, Gross, PRL 110, 263001 (2013).

TT 38.2 Tue 11:00 MA 004

Towards First-Principles Modeling of Electrolytic Solvent Effects in Photo-Catalytic Water Splitting — •Stefan Ringe[1], Sebastian Matera[2], Harald Oberhofer[1], and Karsten Reuter[1] — [1]Technische Universität München — [2]Freie Universität Berlin

Due to the complexity of the physical processes underlying photocatalytic surface reactions, ab-initio computational approaches have to overcome major challenges concerning accuracy and computational costs. In particular, an efficient description of electrolytic solvent effects—which are crucial for charge driven reactions—is highly necessary.

We present an implementation of the modified Poisson-Boltzmann (MPB) model in the highly parallel and numerically efficient all-electron DFT code FHI-aims. In contrast to most implicit solvent models, this technique combines nonlinear dielectric solvent response with a statistical description of solvated finite-sized ions. This has been shown to capture a majority of electrochemical solvent effects appearing in heterogeneous photo-catalysis.[1]

We developed a self-consistent function-space oriented solution scheme for Poisson-Boltzmann-like equations which in contrast to common multi-grid solvers is able to exploit the specialized grids and optimized integration schemes of FHI-aims. We demonstrate the approach and its efficiency for the linearized Poisson-Boltzmann equation and a range of molecular systems. Finally, we discuss how the methodology can be employed for the solution of non-linear problems. [1] Kilic,M.S., Bazant, M.Z., *Phys. Rev. E*, *75*, **2007**, 021502.

TT 38.3 Tue 11:15 MA 004

Phonons in Molecular Crystals: The Role of Collective van der Waals Interactions — •Johannes Hoja and Alexandre Tkatchenko — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

By now, it is well established that dispersive van der Waals (vdW) interactions are crucial for the structure and stability of molecular crystals [1]. However, complete understanding of functionality of molecular crystals also requires a predictive description of response to external perturbations. Here we study the role of vdW interactions on phonons in molecular crystals. This subject is important since such low-frequency vibrations can be used to identify for instance drugs, explosives, and different polymorphic forms of molecular crystals. We studied the vibrational spectra of several molecular crystals with density-functional theory, including many-body dispersion interactions (DFT+MBD method). We find that long-range MBD effects can give rise to novel peaks in the phonon density of states [2], which can not be observed with a simple pairwise treatment of vdW interactions. We further discuss the nature of these vibrations and demonstrate a non-trivial connection between collective vdW interactions and entropy of molecular crystals.

[1] L. Kronik, A. Tkatchenko, Acc. Chem. Res. 47, 3208 (2014).
[2] A. M. Reilly, A. Tkatchenko, Phys. Rev. Lett. 113, 055701 (2014).

TT 38.4 Tue 11:30 MA 004

Converged Nuclear Quantum Statistics from Semi-Classical Path Integrals — •Igor Poltavskyi and Alexandre Tkatchenko — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The quantum nature of nuclear motions plays a vital role in the structure, stability, and thermodynamics of molecular systems. The standard approach to take nuclear quantum effects (NQE) into account is the Feynman-Kac imaginary-time path-integral molecular dynamics (PIMD). Conventional PIMD simulations require exceedingly large number of classical subsystems (beads) to accurately capture NQE, resulting in considerable computational cost even at room temperature due to the rather high internal vibrational frequencies of many molecules of interest.

We propose a novel parameter-free form for the PI partition function and estimators to calculate converged thermodynamic averages. Our approach requires the same ingredients as the conventional PIMD simulations, but decreases the number of required beads by roughly an order of magnitude. This greatly extends the applicability of *ab initio* PIMD for realistic molecular systems. The developed method has been applied to study the thermodynamics of N_2, H_2O, CO_2, and C_6H_6 molecules. For all of the considered systems at room temperature, 4 to 8 beads are enough to recover the NQE contribution to the

total energy within 2% of the fully converged quantum result.

TT 38.5 Tue 11:45 MA 004

Can we get reliable quantum dynamics simulations for vibrational spectra in the condensed phase? — •Mariana Rossi[1], David Manolopoulos[1], and Michele Ceriotti[2] — [1]University of Oxford, Oxford, UK — [2]EPFL, Lausanne, Switzerland

At the level of accuracy we can now achieve in first-principles calculations, the inclusion of more subtle nuclear quantum effects (NQE) in simulations become more relevant. However, their inclusion is challenging for anharmonic and dynamical processes, in particular in the condensed phase. We show a new method to approximate quantum corrections in time-dependent properties based on a path integral framework, called thermostatted ring polymer molecular dynamics (TRPMD) [1], which is immune to pathological problems of previously proposed methods. We perform a systematic comparison of TRPMD with other approaches that rely on different approximations to quantum dynamics, to assess their performance for the IR spectrum of HOD in D_2O and water at different phases/temperatures [2]. Using an empirical potential energy surface (q-TIP4P/f), we find that the different techniques are largely consistent with one another, within a few tens of cm^{-1}. Comparison with classical molecular dynamics demonstrates the importance of NQE even up to 600K. The cross validation between these different approaches provides clues to limitations of their underlying approximations and paves the way for more reliable approaches to nuclear quantum dynamics that are feasible together with electronic structure methods. [1] M. Rossi, M. Ceriotti, D. Manolopoulos, JCP 140, 234116 (2014); [2] M. Rossi, et al., JCP 141, 181101 (2014)

TT 38.6 Tue 12:00 MA 004

Ultra-high temperature properties of ZrC: a fully-anharmonic ab-initio approach — •Andrew Duff[1], Dominique Korbmacher[2], Albert Glensk[2], Blazej Grabowski[2], Joerg Neugebauer[2], and Mike Finnis[1] — [1]Department of Physics and Department of Materials, Thomas Young Centre, Imperial College London, Exhibition Road, London SW7 2AZ, UK — [2]Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf 40237, Germany

As a binary end-member of many of the technologically highly interesting MAX phases, as well a useful refractory material in its own right, there is much to be gained from achieving a more accurate first-principles assessment of the behaviour of ZrC at ultra-high temperatures. Exploiting recent developments in finite-temperature density functional theory (DFT) calculations, we provide valuable data at temperatures where the available experimental data is of low accuracy. Within the framework of the UP-TILD approach [Grabowski 2007], the thermal expansion and heat-capacity of ZrC are calculated up to the melting-point. These fully anharmonic results are compared to calculations performed within the widely used quasi-harmonic approximation (QHA), which treats anharmonic effects in only an approximate manner. Sizeable deviations are found close to the melting point, consistent with the strongly anharmonic lattice vibrations present at such temperatures.

TT 38.7 Tue 12:15 MA 004

Quo vadis electronic friction? Assessing vibrational lifetimes beyond the independent atom approximation — •Simon P. Rittmeyer[1], J. Iñaki Juaristi[2], Jörg Meyer[3], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Depto. & Centro de Física de Materiales (CSIC-UPV/EHU), San Sebastián, Spain — [3]Leiden University, Leiden, The Netherlands

The quest for a both accurate and numerically efficient first-principles-based treatment of electronically non-adiabatic adsorbate dynamics on metal surfaces is still ongoing. A promising candidate in this regard is the concept of electronic friction within the local density friction approximation (LDFA). The numerical efficiency of this approach stems from an intrinsic decomposition and mapping of the interacting system to independent atoms individually embedded in a free electron gas. This inherent simplicity has raised serious conceptual concerns about the accuracy of this theory. On the other hand, it is not clear how much these approximations actually affect the description of "real" observables. In this regard, vibrational lifetimes of high-frequency adsorbate modes on metal surfaces provide a sensitive measure to gauge a non-adiabatic theory. We thus target this observable applying the LDFA for several well-studied systems and discuss it by comparing the results to other theoretical approaches as well as experimental data. Moreover, we present a simple and computationally efficient strategy to extend the LDFA beyond the yet indispensable frozen-surface and independent-atom approximation.

TT 38.8 Tue 12:30 MA 004

Polynomial-oriented linear least squares fits of potential energy surfaces for quantum dynamics — •Florian Habecker and Thorsten Klüner — Universität Oldenburg, Germany

The field TD-QM Molecular Dynamics is facing two major problems within the BO-approximation: I. Solution of the TISE for the electrons and II. Solution of the TDSE for the nuclei. Electronic structure calculations result in a K-dimensional PES (K: number of d.f. for the nuclei) on which the motion of the nuclei is simulated, subsequently.

For economical reasons, the number of sampling points calculated by QC methods is generally smaller than those needed in the QD calculation. Hence, an interface is required to link the two major tasks. Taking the scalar energies E with the corresponding geometry parameters as input, the output of such an interface is a function to calculate any points of the PES, i.e. interpolated and extrapolated values.

Following classical papers on H_3^+ [1 and refs. therein], the linear model function was chosen as a K-dimensional polynomial in this study. The lack of flexibility in this uniform ansatz was restored using appropriate non-linear variable transformations. Applying the method of LLS, precise fits can be calculated in a single non-iterative step. The capability of this approach was validated with a set of 7942 ab initio data points from a 3-D PES of a $CO/Ti_9O_{18}Mg_7^{14+}$-system [2]. Precise fits with chemical accuracy and better have been obtained for moderate expansions of the model function.

[1] W. Meyer, P. Botschwina, P. Burton, *J. Chem. Phys.* **84**, 891 (1986).
[2] H. Spieker, T. Klüner, *Phys. Chem. Chem. Phys.* **16**, 18743 (2014).

TT 38.9 Tue 12:45 MA 004

Representing Complex Potential Energy Surfaces by Artificial Neural Networks — •Christopher Handley and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universit*at Bochum, D-44780 Bochum, Germany

Computer simulations of large systems are computationally costly, and in many cases intractable, when using ab initio methods. More efficient potentials are typically based on approximations specific for particular atomic interactions, and the fitting of these potentials is not straightforward. Neural Networks (NNs) can provide interatomic potentials that are comparable to the accuracy of quantum mechanical calculations [1,2]. They are flexible enough to fit complex functions to quantum mechanical training data and yield accurate energies and forces. Here, we present our recent work towards more transferable NN potentials. [1] C. M. Handley and P. L. A. Poplier, J. Phys. Chem. A, 114, 3371- 3383, (2010). [2] J. Behler, PCCP, 13, 17901-18232 (2011).

TT 38.10 Tue 13:00 MA 004

Kinetic Monte Carlo simulations of thin film growth with anisotropic particles — •Miriam Klopotek, Martin Oettel, and Frank Schreiber — Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Thin film growth is a topic of fundamental experimental research, in particular for organic molecules with semiconducting properties. Thin films of organic molecules are composed of multiple 'imperfect' layers of the molecules, and the structures formed are of fundamental interest for various applications. Organic molecules are mostly highly anisotropic, rendering complex ordering at various length- and timescales within the growing film that is not seen in the case of isotropic molecular/atomistic films [1]. We explore how this particle anisotropy affects the growth dynamics by means of computer simulations. We have developed a novel algorithm to simulate large-scale thin film growth with rod-like particles using an accelerated Monte Carlo technique called *kinetic Monte Carlo* [2]. We disuss the simulations and the most relevant findings arising from statistical observables related to the orientational order of the rods. To relate the non-equilibrium growth structures to equilibrium we performed equilibrium calculations of a single layer of rods, as well. [1] S. Kowarik, A. Gerlach, S. Sellner, F. Schreiber, L. Cavalcanti, and O. Konovalov. Real-time observation of structural and orientational transitions during growth of organic thin films. *Phys. Rev. Lett.*, 96:125504, March 2006. [2] Andrea C. Levi and Miroslav Kotrla. Theory and simulation of crystal growth. *Journal of Physics: Condensed Matter*, 9(2):299, 1997.

TT 38.11 Tue 13:15 MA 004

Ti and N adatom diffusion on, and N_2 desorption from TiN(001) surfaces via *ab initio* and classical molecular dy-

namics — •Davide G. Sangiovanni[1], Daniel Edström[1], Lars Hultman[1], Ivan Petrov[1,2], Valeriu Chirita[1], and Joe E. Greene[1,2] — [1]Thin Film Physics, IFM, Linköping University, Sweden — [2]University of Illinois, Urbana-Champaign, Illinois, USA

We use classical and *ab initio* molecular dynamics to investigate fundamental atomistic processes and surface properties responsible for TiN surface evolution during thin film growth. The rate of adatom migration and N_2 desorption events are determined as a function of temperature to extract activation energies, attempt frequencies, and diffusion coefficients. Ti adatoms (Ti_{ad}), highly mobile on TiN(001) terraces, diffuse among fourfold hollow sites, primarily along <100> channels via single and long jumps. Ti_{ad} jumps on TiN(001) are highly correlated; an effect which leads to smaller diffusion coefficients than those determined via adatom random walks. Due to strong bonds formed with underlying N surface (N_{surf}) atoms, N adatoms (N_{ad}) are considerably less mobile on TiN(001) than Ti adatoms. After several N_{ad}/N_{surf}-pair exchange reactions, with very few N_{ad} jumps among neighboring stable surface sites, the N_{ad}/N_{surf} pair desorbs, leaving an anion surface vacancy which acts, in turn, as a catalyst for N_2 dissociative chemisorption. This pathway for N_2 desorption from TiN(001) is considerably more probable than N adatom recombination, which is kinetically hindered due to short-range N_{ad}/N_{ad} repulsive interactions.

TT 39: Graphene: Growth & Intercalation (jointly with O, HL)

Time: Tuesday 10:30–13:00 Location: MA 041

TT 39.1 Tue 10:30 MA 041

First-principles Study of the Origin of a Rippled Graphene Phase on Ir(001) — •Mighfar Imam[1], Natasa Stojic[1,2], and Nadia Binggeli[1,2] — [1]The Abdus Salam International Centre for Theoretical Physics Strada Costiera 11, 34151 Trieste, Italy — [2]IOM-CNR Democritos, Trieste, I-34151, Italy

An interesting graphene phase on Ir(001) comprising ordered one-dimensional ripples of nanometer periodicity with exceptionally large buckling has recently been observed experimentally [1]. In this phase, chemisorbed lines of graphene, only a few nanometers wide, strongly bind to the substrate along Ir[010], while the whole graphene film markedly buckles between these periodic lines, resulting in graphene ripples along Ir[100]. We have performed a density functional theory study including the long range van der Waals interactions to investigate the microscopic mechanisms responsible for the formation of this new graphene phase on Ir(001). With our calculated trends of the chemisorption and rippling energies, we explain the appearance of a buckled chemisorbed phase with a specific nanometer periodicity. We have also analyzed the effect of changing graphene curvature on its electronic structure and chemisorption energy, finding a new feature in the conduction band close to the Fermi energy. This new feature in the conduction states is identified as the one largely responsible for the strong local chemisorption of graphene.

[1] A. Locatelli et al., ACS Nano, 7, 6955 (2013)

TT 39.2 Tue 10:45 MA 041

Graphene induced faceting of Ir(557) — Christian Witt, Michael Horn-von Hoegen, and •Frank-J. Meyer zu Heringdorf — University Duisburg-Essen, Faculty for Physics and CENIDE, Lotharstrasse 1, 47057 Duisburg

With its great application potential due to the unique electronic structure and the mechanical properties, graphene holds promise for future carbon-based device architectures. Lately, a lot of effort has been invested into the growth of graphene on metal surfaces, due to the possibility to separate the graphene from the surface after growth. In some cases, however the interaction between graphene and the substrate, in conjunction with the elevated sample temperatures, results in a modification of the substrate surface morphology during growth. Here we investigate the modification of a regularily stepped Ir(557) surface during catalytic growth of graphene at various ethylene pressures and temperatures with low energy electron microscopy. Ir(557) is a vicinal (111) surface with a miscut of 9.45° in [001] direction. We find simultaneous growth of graphene flakes and nano-ribbons, depending on ethylene pressure and sample temperature. The nano-ribbons grow exclusively along the steps. Both, flakes and nano-ribbons, induce a faceting of the surface during growth. An intercalation of oxygen between the graphene and the faceted surface does not affect the already present facets. The orientation of the facets were determined by reciprocal space mapping and (ex-situ) AFM measurements.

TT 39.3 Tue 11:00 MA 041

Comparing graphene growth on Cu(111) vs. oxidized Cu(111) — Stefano Gottardi[1], Kathrin Müller[1], Luca Bignardi[1], Juan Carlos Moreno Lopez[1], Tuan Anh Pham[1], Alexei Barinov[2], Jonas Björk[3], Petra Rudolf[1], and •Meike Stöhr[1] — [1]University of Groningen — [2]Sincrotrone Trieste — [3]Linköping University

The epitaxial growth of graphene on catalytically active metallic surfaces via chemical vapor deposition (CVD) is known to be one of the most reliable routes towards high quality large-area graphene. This CVD-grown graphene is generally coupled to its metallic support resulting in a modification of its intrinsic properties. Growth on oxides is a promising alternative that might lead to a decoupled graphene layer. Here, we compare graphene on a pure metallic to graphene on an oxidized copper surface, in both cases grown by a single step CVD process under similar conditions. Remarkably, the growth on copper oxide - a high-k dielectric material - preserves the intrinsic properties of graphene; it is not doped and a linear dispersion is observed close to the Fermi energy. Density functional theory calculations give additional insight into the reaction processes and help explaining the catalytic activity of the copper oxide surface.

TT 39.4 Tue 11:15 MA 041

Ir(111) surface state stability against Li adsorption: role of graphene — •Petar Pervan[1], Ivo Pletikosić[2], Marin Petrović[1], Iva Šrut Rakić[1], Marko Kralj[1], Milorad Milun[1], Tonica Valla[2], and Predrag Lazić[3] — [1]Institut za fiziku, Bijenička 46, 10000 Zagreb, Croatia — [2]Department of Condensed Matter Physics & Materials Science, Brookhaven National Lab, Upton — [3]Institut Rudjer Bošković, Bijenička 54, 10000 Zagreb, Croatia

Surface states (SS) are known to be extremely sensitive to the presence of defects or adsorbates with the effect that any surface state would disappear in response to submonolayer coverage of adsorbates. Moreover, adsorbates can induce a change of the surface potential which in turn may strongly affect its binding energy. In this work we report on the Li intercalation of graphene on Ir(111) and its influence on the Ir surface state at the K point studied by means of the Low Energy Electron Diffraction (LEED), the Angle Resolved Photoemission Spectroscopy (ARPES) and the Density Functional Theory (DFT). We have found that at all stages of the Li intercalation the integrity of the surface state at the K point has been preserved. Despite the increase of the SS binding energy its spectral intensity and the width were constant at all Li concentrations. This finding suggests an unperturbed surface state coherence at the K point. Away from the K point the surface state exhibits strong hybridization with graphene pi bands which is accompanied by the opening of the band gap at higher binding energy with respect to the hybridisation point.

TT 39.5 Tue 11:30 MA 041

Chemical Functionalization of Graphene via Hyperthermal Molecular Reaction — Girjesh Dubey[1], Roberto Urcuyo[1], Sabine Abb[1], Gordon Rinke[1], Marko Burghard[1], •Stephan Rauschenbach[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Institut de Physique de la Matière Condensée, EPFL, Lausanne, Switzerland

Covalent functionalization represents a viable pathway for tailoring graphene's electronic properties, for instance to open a band-gap. It furthermore enables subsequent chemical coupling for applications in molecular diagnostics and molecular electronics. In this study, chemical vapor deposited (CVD) graphene is covalently functionalized though electrospray ion beam deposition (ES-IBD) of hyperthermal molecular cation beams of 4,4-azobis(pyridine). The one-step, room temperature ion-surface reaction process takes place in high vacuum (10^{-7} mbar), and requires a threshold kinetic energy of 165 eV of the molecular ions. The covalent attachment of the molecules is proven by the effect of thermal annealing, which removes the intense D peak

in the Raman spectrum of the functionalized graphene. Based up X-ray photoelectron spectroscopy data, we conclude that the attached species are azopyridinium groups. A high functionalization degree of 3% of the carbon atoms of graphene is attained after 3-5 hours of ion exposure of 2×10^{14} azopyridinium/cm^2 of which 50% bind covalently.

G. Dubey et al.: *J. Am. Chem. Soc.* **136**, 13482-13485 (2014)

TT 39.6 Tue 11:45 MA 041

Quantum interference on the doped graphene/SiC systems — •Mykola Telychko[1], Pablo Merino[2], Pingo Mutombo[1], Martin Ondračeк[1], Prokop Hapala[1], Oleksandr Stetsovych[1], Martin Švec[1], and Pavel Jelínek[1] — [1]Institute of Physics ASCR, Cukrovarnicka 10, Praha, Czech Republic — [2]Max Planck Institute for Solid State Research, Heisenberg Strasse 1, 705669 Stuttgart

We report methodology for co-doping of epitaxial graphene grown on the SiC(0001) substrate by boron and nitrogen atoms. Nitrogen doping was achieved using direct nitrogen ion implantation into the graphene lattice and subsequent thermal stabilization. Boron doping was achieved by introducing the additional source of boron atoms during growth process of the graphene/SiC(0001).

Atomically-resolved low-temperature STM/AFM measurements of well-defined single substitutional nitrogen and boron dopants reveal that nitrogen dopants in graphene lattice feature a strong destructive quantum interference effect, tunable by changing the tip-sample separation. The current dependence on the tip position is successfully modelled by DFT and STM simulations for the both types of dopants. Absence of the destructive interference over the boron dopants allows clear chemical discrimination between the N and B atoms.

TT 39.7 Tue 12:00 MA 041

Scanning Tunneling Microscopy of epitaxial Graphene with single ion-implanted Boron, Nitrogen and Carbon atoms — •Philip Willke[1], Anna Sinterhauf[1], Julian Amani[2], Sangeeta Thakur[3], Thomas Kotzott[1], Steffen Weikert[2], Kalobaran Maiti[3], Hans Hofsäss[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Universität Göttingen, Germany — [2]II. Physikalisches Institut, Universität Göttingen, Germany — [3]Department of Condensed Matter Physics and Materials' Science, TIFR, Mumbai, India

Using scanning tunneling microscopy and spectroscopy we investigate the structural and electronic properties of single substitutional atoms in SiC-graphene. These are prepared by low-energy ion implantation, which we use as a suitable method for boron and nitrogen incorporation in graphene [1,2]. We find, that boron and nitrogen atoms lead to an effective doping of the graphene sheet and allow to reduce or raise the position of the Fermi level, respectively. The electronic properties of the doping atoms are additionally addressed. To reveal the defect creation in the doping process $^{12}C^+$ carbon ions, that only introduce defects and no impurity atoms, are studied as a reference. Moreover, we perform magnetotransport measurements to investigate the influence of the microscopic structure on the graphene transport properties. This work was supported by DFG priority program 1459 "Graphene".

[1] P. Willke et al., Appl. Phys. Lett. 105, 111605 (2014)
[2] U. Bangert et al., Nano Lett. 13(10) (2013)

TT 39.8 Tue 12:15 MA 041

Reversible Hydrogenation of Graphene on Ni(111) - Synthesis of 'Graphone' — •Julian Gebhardt[1], Wei Zhao[2], Florian Späth[2], Karin Gotterbarm[2], Christoph Gleichweit[2], Hans-Peter Steinrück[2], and Andreas Görling[1] — [1]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Understanding the adsorption and reaction between hydrogen and graphene is of fundamental importance for developing graphene-based concepts for hydrogen storage and for the chemical functionalization of graphene by hydrogenation. Recently, theoretical studies of single-sided hydrogenated graphene, so called graphone, predicted it to be a promising semiconductor for applications in graphene-based electronics. Here, we report on the synthesis of graphone bound to a Ni(111) surface. We investigate the formation process by X-ray photoelectron spectroscopy (XPS), temperature-programmed desorption (TPD), and density-functional theory calculations, showing that the hydrogenation of graphene with atomic hydrogen indeed leads to graphone, i.e., a hydrogen coverage of 1 ML (4.2 wt%). In addition, the dehydrogenation of graphone was shown to be possible by XPS and TPD measurements. The complex desorption process was attributed to coverage-dependent changes in the activation energies for the associative desorption of hydrogen as molecular H_2.

TT 39.9 Tue 12:30 MA 041

Towards Understanding the Wetting of Nanostructured Surfaces — •Mausumi Chattopadhyaya and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Berlin, Germany

Water is arguably the most important liquid. Understanding how water interacts with nanostructures leads to many fundamental questions both in theory and experiment. On the experimental side, it has been widely quoted that the contact angle of water on graphite is in the range of 90°-95°. However, careful measurements using ultra high vacuum techniques lead to drastically different values of 35±4°. From theory point of view, a precise description of water interacting with nanostructured surfaces seems to require the highest levels of correlated quantum-chemical methods. Here, we study the interaction of water with layered materials with the aim to determine the contact angle of water on different nanostructured surfaces. This demands a precise calculation of the surface energy of the nanostructure and the interaction energy between water and the surface. We have carried out systematic calculations of water interacting with few-layer graphene and h-BN surfaces. These calculations have been done using pairwise Tkatchenko-Scheffler(TS) scheme and many-body dispersion (MBD) method within density functional theory (DFT). Remarkably, our results suggest that the binding energy of a water molecule does not depend on the number of graphene or h-BN layers. We finally discuss the current work aiming to understand the contact angle of water on a range of nanostructured surfaces.

TT 39.10 Tue 12:45 MA 041

Fingerprinting graphene: self-assembly by breaking the rules of surface science — •Samuel Grandthyll[1], Stefan Gsell[2], Michael Weinl[2], Matthias Schreck[2], Karin Jacobs[1], and Frank Müller[1] — [1]Saarland University, Experimental Physics, 66041 Saarbruecken, Germany — [2]University of Augsburg, Experimental Physics 4, 86135 Augsburg, Germany

Epitaxial graphene is expected to be the only synthesis route to obtain large-area sheets of this silicon substitute for the engineering of future nano electronic devices on an industrial scale. So far, there are different recipes to obtain epitaxial graphene, using either intrinsic carbon, as released by the selective desorption of silicon from a SiC surface, or using extrinsic carbon, as via the chemical vapor deposition (CVD) of simple hydrocarbons on transition metal surfaces. In addition, even ex-situ deposition of liquid precursors (LPD) provides well-ordered graphene monolayers. In order to explore the limits of self-assembly in LPD synthesis, we show that graphene formation on transition metal surfaces is an extraordinarily robust mechanism that also works when carbon is provided in the maximal undefined way, namely by using a human fingerprint as a precursor. Our results show that "fingerprinting" graphene provides well-ordered monolayers of the same quality as in case of using ultrapure synthetic single precursors. The unique directedness of the self-assembly process of graphene on transition metals by liquid precursor deposition therefore offers a simple synthesis route for epitaxial graphene [1].

[1] F. Müller et al., Langmuir 30 (2014), 6114-6119

TT 40: Electronic Structure of Magnetism, Micromagnetism, Computational Magnetism (organized by MA)

Time: Tuesday 9:30–12:30 Location: H 0112

TT 40.1 Tue 9:30 H 0112

Spin-orbit coupling effects on spin-dependent inelastic electronic lifetimes in ferromagnets — •Dennis Nenno, Steffen Kaltenborn, and Hans Christian Schneider — Physics Department and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern

We present results for spin-dependent inelastic electronic lifetimes in the 3d ferromagnets iron, cobalt, and nickel due to carrier-carrier Coulomb interactions including spin-orbit coupling in the band structure and in the wave functions. Including the spin-orbit interaction in the electronic wave functions presents an important step towards the resolution of a long standing discrepancy between theoretical and experimental results for spin-dependent electronic lifetimes. This subject has recently received renewed attention due to its importance for hot-electron spin transport [1]. Our approach is based on density functional theory and an accurately determined dielectric function [2]. With this numerical framework we find that the spin-dependent density of states at the Fermi energy does not, in general, determine the spin dependence of the lifetimes because of the effective spin-flip transitions allowed by the spin mixing [3]. Thus, the majority and minority electron lifetimes computed including spin-orbit coupling for these three 3d ferromagnets do not differ by more than a factor of 2, and agree with experimental results.

[1] M. Battiato, K. Carva, and P. M. Oppeneer, PRB 86, 024404 (2012). [2] S. Kaltenborn and H. C. Schneider, PRB 88, 045124 (2013). [3] S. Kaltenborn and H. C. Schneider, PRB 90, 201104(R) (2014).

TT 40.2 Tue 9:45 H 0112

Systematic derivation of an effective spin-Hamiltonian based on a modified multi-orbital Hubbard model — •Markus Hoffmann and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Theoretical descriptions of magnetic ground states, dynamical or thermodynamical properties of magnetic systems are often achieved through a multi-scale approach: DFT calculations are mapped onto a lattice spin-Hamiltonian whose properties are then evaluated carrying out Monte-Carlo or spin-dynamic simulations. For many bulk materials, the well-known Heisenberg exchange provides a sufficient description of the properties, whereas at surfaces or thin films occasionally so-called higher-order exchange interactions play a significant role. Those interactions are motivated from a single-band Hubbard model of a spin $S = 1/2$ system. However, typical magnetic moments at surfaces are in the order of 2 or 3 μ_B equivalent to $S = 1$ or $S = 3/2$. In this contribution, we present a systematic derivation of effective lattice spin-Hamiltonians based on a rotational invariant multi-orbital Hubbard model including a term ensuring Hund's rule coupling. The model is derived down-folding the degree of freedom into the proper low-energy spin sector using Löwdin's partitioning. Up to fourth order perturbation we found for $S \geq 1$ beyond the conventional Heisenberg term a biquadratic, 3-spin and 4-spin interaction. We show that the so-far not considered 3-spin interaction explains the puzzling energy spectrum of the magnetic states for a single Fe monolayer on Rh(111).

TT 40.3 Tue 10:00 H 0112

Navigation on the energy surface of the noncollinear Alexander-Anderson model using a magnetic force theorem — •Pavel Bessarab[1,2], Valery Uzdin[2,3], and Hannes Jónsson[4,5] — [1]Royal Institute of Technology KTH, Stockholm, Sweden — [2]St. Petersburg State University, St. Petersburg, Russia — [3]St. Petersburg National Research University of Information Technologies, Mechanics and Optics, St. Petersburg, Russia — [4]University of Iceland, Reykjavik, Iceland — [5]Aalto University, Espoo, Finland

Magnetic force theorem is derived within the multiple impurity, noncollinear Alexander-Anderson (NCAA) model - an important tool for efficient calculation of the total energy gradient with respect to orientation of magnetic moments, the magnetic 'forces'. Efficient evaluation of magnetic forces is of great importance for the large scale simulation of spin dynamics, minimization of the energy to identify stable and metastable magnetic states, or, in general, navigation on the energy surface of a magnetic system. NCAA model and magnetic force theorem are applied to calculate minimum energy paths between stable magnetic states of the monolayer Fe clusters on a W(110) surface, revealing complex mechanism of the magnetization reversal. Moreover, a noncollinear magnetic state is identified in a 7 x 7 atomic row Fe island where the magnetic moments are arranged in an antivortex configuration with the central ones pointing out of the (110) plane. The minimum energy path between this antivortex state and the collinear ground state is also calculated and the thermal stability of the antivortex state estimated.

TT 40.4 Tue 10:15 H 0112

Non-harmonic quantum dynamics of single spin systems — •Mario Krizanac, David Altwein, Elena Vedmedenko, and Roland Wiesendanger — Institute of Applied Physics and Interdisciplinary Nanoscience Center Hamburg , Germany

The time evolution of single quantum spins became accessible to the experimental observation in the last years [J. Phys. D:Appl. Phys.44(2011)]. Therefore, it was our motivation to study the dynamics of single quantum spin systems with uniaxial anisotropy in an external magnetic Bz-field from a theoretical perspective within the Schroedinger formalism. It has been found that the spin dynamics shows a very complicated non-harmonic periodicity. The period depends on the ratio of the external magnetic Bz-field and the uniaxial anisotropy in Sz direction. We observed two cases, the first one of very high periodicity and a second one of low periodicity. The conditions for these cases can be formulated in the form of a simple equation, which can be easily generalized to describe these conditions for single quantum spin systems of any size.

Atomic magnetism revealed by spin-resolved scanning tunnelling spectroscopy [J. Phys. D: Appl. Phys.44(2011)] Jens Wiebe, Lihui Zhou and Roland Wiesendanger Institute of Applied Physics, Hamburg University, Jungiusstrasse 11, D-20355 Hamburg, Germany

TT 40.5 Tue 10:30 H 0112

Real-time dynamics of a classical spin exchange coupled to a Fermi sea — •Mohammad Sayad and Michael Potthoff — I. Institut für Theoretische Physik , University of Hamburg, Germany

Using a numerical time-step propagation technique, we study the real-time dynamics of a single classical spin locally coupled via an antiferromagnetic exchange J to a system of non-interacting electrons. The dynamics is initiated by suddenly switching a local magnetic field B. In the regime of weak J and B, linear-response theory and the separation of time scales can be employed to derive the Landau-Lifshitz-Gilbert equation. We show, however, that this theory must break down and that the Gilbert damping becomes ill-defined in the case of one-dimensional systems. The reversal time of the spin is systematically calculated in the entire parameter regime. For strong J we find an incomplete relaxation on a short time scale followed by a slow drift towards saturation. Retardation effects and deviations from adiabatic spin dynamics are discussed for systems with a single and with two classical spins.

15 min. break

TT 40.6 Tue 11:00 H 0112

Finite temperature and magnetic field transport in 1D quantum magnets — •Xenophon Zotos — Physics Department - University of Crete — Crete Center for Quantum Complexity and Nanotechnology — FORTH - IESL

I'll present recent exact results on the finite temperature and magnetic field magneto-thermal transport in the one dimensional spin-1/2 Heisenberg model obtained using the Bethe ansatz (BA) method. In particular, I'll discuss the behavior of spin Drude weight as a function of magnetic field down to low temperatures. These new results are based on a previous analysis by the author of the spin Drude weight in zero magnetic field.

Furthermore, I'll discuss the thermodynamics, thermal transport and dynamics (ESR), of the spin S=1 easy-plane quasi-one dimensional quantum magnet NiCl2-4SC(NH2)2 (DTN). The analysis is based on an effective spin-1/2 anisotropic (s= 1/2) Heisenberg model description that is put on a firm basis by comparing the thermodynamics of

the S=1 model, obtained using TMRG, with exact BA specific heat and magnetisation results for the s=1/2 Heisenberg model. For the thermal conductivity in a magnetic field, Ill compare numerical data on the S=1 model obtained using exact diagonalization techniques to exact results using the BA method. For the ESR data, using a recently developed BA technique, I'll show that the extremely sharp line observed in experiments, is due to a singular excitation to a single excited state.

TT 40.7 Tue 11:15 H 0112

Multi-scale modelling of magnetization dynamics — •Andrea De Lucia, Mathias Kläui, and Bejnamin Krüger — Institut für Physik, Johannes Gutenberg Universität, Mainz

A Multi-scale Magnetization Dynamics Simulation scheme was developed and applied to systems with special spin structures and properties. The MicroMagnum simulator was used as starting point and expanded to include a Multi-scale approach. The software selectively simulates different regions of a ferromagnetic sample employing the most suitable discretization and model according to the properties of each region. Simulating magnetization dynamics in a Multi-scale environment allows one to rapidly evaluate the Landau-Lifshitz-Gilbert equation in a mesoscopic sample with nanoscopic accuracy where needed. Possible application of this software include Skyrmion Dynamics, Domain Wall motion and Spin Wave generation.

TT 40.8 Tue 11:30 H 0112

Effective models for exchange bias systems based on atomistic spin dynamics simulations — •Irina Stockem, Stefan Muschack, and Christian Schröder — Bielefeld Institute for Applied Materials Research, University of Applied Sciences Bielefeld, Wilhelm-Bertelsmann-Str. 10, 33602 Bielefeld, Germany

The exchange bias anisotropy was observed at stacked ferromagnetic and antiferromagnetic layers by Meiklejohn and Bean in the 1950$^{\text{th}}$ [1]. The exchange bias leads to an asymmetric shift of the hysteresis loop, which is fixed during the fabrication process in conventional systems. In novel systems, like Co/Cr_2O_3, this shift can be switched [2]. Although the discovery of the exchange bias is more than half a century ago a comprehensive theoretical model is still missing. Many simplified and analytical solvable models exist but these are not applicable to real exchange biased structures. In order to obtain a better understanding of the dominating factors of exchange bias systems we have developed effective models and investigated these by spin dynamics simulations [3]. We compare our results to existing models and to atomistic spin dynamics simulations of a three dimensional Co/Cr_2O_3 model system.

[1] W. H. Meiklejohn and C. P. Bean, Phys. Rev. **105**, 904 (1957).
[2] Y. Shiratsuchi et al., Appl. Phys. Lett. **100**, 262413 (2012).
[3] L. Engelhardt and C. Schröder, in Molecular Cluster Magnets, World Scientific Publishers, Singapore (2011).

TT 40.9 Tue 11:45 H 0112

Simulation of coercivities and magnetization reversal mechanisms in fourfold ferromagnetic systems of different dimensions and orientations — •Tomasz Blachowicz[1] and Andrea Ehrmann[2] — [1]Silesian University of Technology, Institute of Physics, Poland — [2]Niederrhein University of Applied Sciences, Faculty of Textile and Clothing Technology, Germany

The stability of magnetic states during magnetization reversal, especially at remanence, belongs to the important issues in examination of magnetic nanosamples. Our presentation gives an overview of different fourfold magnetic wire systems, simulated by Magpar. Wire lengths have been chosen from 30 nm to 70 nm, while the single wires have length-to-diameter ratios between 3 and 11. Simulations have been carried out for angular in-plane directions of the externally applied field from 0° (parallel to one pair of wires) to 45°. Depending on system dimensions and external field angle, different magnetization reversal mechanisms could be observed as well as changes between stable and instable magnetic states [1].

Intermediate states at vanishing external field, reached by minor loops starting at steps in the hysteresis loop, are of special interest for application in novel data storage media systems. The presentation shows different possibilities to create such states and examines their stability by comparing hysteresis loops, special distribution of magnetization, and exchange energy as function of the externally applied field for a number of sample dimensions and external field angles.

[1] T. Blachowicz, A. Ehrmann, J. Appl. Phys. 113, 013901 (2013)

TT 40.10 Tue 12:00 H 0112

Micromagnetic analysis of nucleation and pinning processes in supermagnets — Dagmar Goll[1], Therese Dragon[2], Matthias Katter[3], and •Helmut Kronmueller[2] — [1]Aalen University, Materials Research Institute (IMFAA), Aalen — [2]Max Planck Institute for Intelligent Systems — [3]Vacuumschmelze GmbH & Co. KG, Hanau

The large discrepancy between theoretical predictions and realized magnetic properties of hysteresis loops of high-quality permanent magnets, known as Brown-paradox, has been the matter of discussions over decades of years. In particular whether the leading hardening mechanism is due to a nucleation mechanism or to domain wall pinning has been the topic of many publications with contrary statements. Here the existence of single or multi-domain grains plays a central role. This contribution presents the following basic results which allow a distinction between the two types of hardening mechanisms: 1. Coercive field H_c as a function of maximum applied magnetic field. 2. Change of domain patterns as a function of applied magnetic field. 3. Angular dependence of H_c. 4. Temperature dependence of H_c. Experimental results obtained for nanocrystalline systems of FePt and MnBi and sintered Nd-Fe-B based permanent magnets are compared with micromagnetic analytical results. It is shown that for high-quality permanent magnets the dominant hardening mechanism corresponds to the nucleation process.

TT 40.11 Tue 12:15 H 0112

Nonlinear frequency-dependent effects in the dc magnetization of uniaxial magnetic nanoparticles in superimposed strong alternating current and direct current fields — •William Coffey[1], Nijun Wei[1], Sergey Titov[1], Yuri Kalmykov[2], and Declan Byrne[1] — [1]Department of Electronic and Electrical Engineering, Trinity College, Dublin 2, Ireland — [2]Université de Perpignan Via Domitia, Laboratoire de Mathématiques et Physique, F-66860, Perpignan, France

The dc component of the magnetization of noninteracting fine magnetic particles possessing simple uniaxial anisotropy and subjected to strong ac and dc bias magnetic fields is calculated via the magnetic Langevin equation. In the presence of an ac driving field, the dc component of the magnetization of uniaxial particles alters drastically leading to new nonlinear effects; in particular, it becomes frequency-dependent. In axial symmetry, where the strong ac field is parallel to the easy axis of a particle, two distinct dispersion regions in the dc magnetization at low and mid-frequencies emerge, corresponding to longitudinal overbarrier and intrawell relaxation modes. Such frequency-dependent behavior allows one to estimate the magnetization reversal time via the half-width of the low-frequency dispersion band. Otherwise, by applying the strong ac field at an angle to the easy axis of a particle so breaking the axial symmetry, a third high-frequency nonlinear resonant dispersion in the dc component of the magnetization appears accompanied by parametric resonance behavior due to excitation of transverse modes with frequencies close to the precession frequency.

TT 41: Spintronics: Excitons and Local Spins (jointly with HL, MA)

Time: Tuesday 9:30–11:30 Location: ER 270

TT 41.1 Tue 9:30 ER 270

Transport and manipulation of indirect exciton spins in GaAs double quantum well structures — Adriano Violante, Serkan Büyükköse, Klaus Biermann, and •Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Indirect excitons in double quantum well (DQW) structures are interesting particles for information storage due to the electrically controlled coupling to photons. Here, we report on the coherent control and transport of IX spins in GaAs DQWs using spatially and polarization resolved photoluminescence (PL). We show that optically IXs spins optically excited by a focused, circularly polarized light spot precess around the spin-orbit magnetic field while moving over distances exceeding 20 μm from the excitation spot. The spatial precession frequency depends on the spin transport direction and can be controlled by the bias applied across the DQW structure. From the dependence of the spin dynamics on transport direction, bias, and external magnetic fields we directly determined the Dresselhaus and Rashba electron spin splitting coefficients for the DQW structure. The long *IX* lifetimes, together with the negligible contribution of holes to the spin dynamics, are attributed to spatial separation of the electron and hole wave functions by the electric field, which reduces the electron-hole exchange interaction. If extended to the single exciton regime, the present results imply that IXs can be used as flying spin qubits for application in the quantum information processing.

TT 41.2 Tue 9:45 ER 270

Spin properties of the indirect exciton in indirect band-gap (In,Al)As/AlAs quantum dot ensembles — •Jörg Debus[1], Victor F. Sapega[2], Timur S. Shamirzaev[3], Daniel Dunker[1], Evgeny L. Ivchenko[2], Dmitri R. Yakovlev[1,2], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, TU Dortmund, Dortmund, Germany — [2]Ioffe Physical-Technical Institute, St. Petersburg, Russia — [3]Institute of Semiconductor Physics, Novosibirsk, Russia

The band structure of type-I (In,Al)As/AlAs quantum dots with band gap energy exceeding 1.63 eV is indirect in momentum space, leading to long-lived exciton states with potential applications in quantum information. Optical access to these excitons is provided by mixing of the Γ- and X-conduction band valleys. We report on spin properties of the indirect exciton studied by time-resolved photoluminescence (TRPL) and resonant spin-flip Raman scattering (SFRS) [1-3]. The SFRS characterizes the Γ-X-valley electron state mixing, provides access to the fine structure of the indirect exciton and enables the preparation of its spin states as well as the determination of the spin-flip mechanisms. From the TRPL we evaluate very long longitudinal spin relaxation times (200 μs at 4 T and 1.8 K) that are rather robust against temperature changes. The temporal evolution of the circular polarization degree of the photoluminescence moreover changes its sign in the μs-range thus hinting at dark and bright indirect excitons contributing by their different spin dynamics. [1] T. S. Shamirzaev et al., Phys. Rev. B **84**, 155318 (2011). [2] D. Dunker et al., Appl. Phys. Lett. **101**, 142108 (2012). [3] J. Debus et al., Phys. Rev. B **90**, 125431 (2014).

TT 41.3 Tue 10:00 ER 270

Coherent control and readout of single spins in silicon carbide — •Matthias Widmann[1], Sang-Yun Lee[1], Torsten Rendler[1], Nguyen Tien-Son[2], Helmut Fedder[1], Erik Janzén[2], and Jörg Wrachtrup[1] — [1]3.Physikalisches Institut, Universität Stuttgart — [2]Department of Physics, Chemistry and Biology, Linköping University

Single spin manipulation is one of the main subjects in research not only for quantum information processing (QIP) but also for quantum metrology. Having isolated spins in solids has advantages of stability and fabrication. Deep level defects in diamond and impurity donors in silicon have been considered as promising candidates and several key steps towards QIP have been achieved. However, there exist disadvantages which have hindered their successful integration into modern electronic devices; cryogenic temperature mandatory for readout of spins in silicon, and difficulty in electrical initialization and readout in diamond. These motivate to investigate other host materials such as silicon carbide (SiC). SiC combines the advantages of silicon and diamond, because electrical detection and optical access of spin ensembles at room temperature (RT) is possible, and it also benefits from modern fabrication techniques. Addressing individual spin states have not been shown yet, however, is highly demanded to set up a base for scalable atomic-scale quantum technologies. By presenting coherent control and readout of single spins in SiC at RT we prove that SiC is a promising platform for the scalable spintronic devices [1]. [1] M. Widmann et al., Coherent control of single spins in silicon carbide at room temperature, to be published in Nature Materials.

TT 41.4 Tue 10:15 ER 270

Nuclear magetic resonance on a single quantum dot — •Gunter Wüst[1], Mathieu Munsch[1], Andreas Kuhlmann[1], Martino Poggio[1], Arne Ludwig[2], Andreas Wieck[2], Dirk Reuter[3], and Richard J Warburton[1] — [1]University of Basel, Switzerland — [2]Ruhr-Universität Bochum, Germany — [3]Universität Paderborn, Germany

The spin coherence of an electron trapped to a GaAs or InGaAs quantum dot is limited by noise in the nuclear spins of the host material [1]. Understanding and controlling the nuclear spins is therefore important for quantum applications. We report here nuclear magnetic resonance (NMR) experiments on the 100,000 nuclear spins that have a contact hyperfine interaction with a quantum dot electron spin [2]. The main technique is to sweep the frequency of an in-plane magnetic field. In this way, all nuclear spins are addressed despite the presence of four main isotopes with different gyromagnetic ratios. The nuclear spins are polarized and read-out via resonant spectroscopy allowing us to reach a sensitivity to about 1,000 nuclear spins. We evidence a plateau in the NMR sweep rate dependence associated to the existence of quadrupole interactions. Detailed analysis allows the quadrupole distributions for each isotope to be determined, along with an effective nuclear spin temperature following polarization (8 mK) and an In concentration (20%). Ongoing experiments determined in addition the Hahn echo coherence times (1 ms) and their dependence on quantum dot charge.

[1] R. J. Warburton et al, Nature Materials 12, 483-493 (2013) [2] M. Munsch, Nature Nanotechnology 9, 671-675 (2014)

TT 41.5 Tue 10:30 ER 270

Distinct Nuclear Spin Signatures in the Spin Noise of Donor Bound Electrons — •Fabian Berski[1], Pavel Sterin[1], Jens Hübner[1], Andreas Wieck[2], and Michael Oestreich[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Ruhr-Universität Bochum, Angewandte Festkörperphysik, Universitätsstr. 150, D-44780 Bochum, Germany

The hyperfine interaction acts as a main source of decoherence for localized electron spins in III-V semiconductor material systems and is thus a challenge for quantum information processing [1]. However, this interaction can also serve as a subtle probe of nuclear dynamics, which manifests itself in the spin dynamics of electrons.

Here, we study an ensemble of non-interacting donor bound electrons (D^0X) in a strain-free, high purity Gallium Arsenide host matrix, and find intriguing features of the nuclear spin dynamics in the electronic spin noise. The ideal tool to study such an interplay is spin noise spectroscopy, since it allows to control the dissipated amount of energy in the system and is a potential quantum non-demolition measurement [2]. However, by selecting the detuning between the D^0X transition and the energy of the used laser light, we find strong evidence for a significant nuclear polarization, even at low laser power, linearly polarized light and vanishingly small transversal magnetic fields.

[1] Chekhovich, et al., Nature Mat. **12**, 6 (2013).
[2] Hübner, et al., Phys Status Solidi B **251**, 1824 (2014).

TT 41.6 Tue 10:45 ER 270

Spin Dynamic of Electrons and Holes in Single Quantum Dots — •Ramin Dahbashi[1], Julia Wiegand[1], Jens Hübner[1], Klaus Pierz[2], Arne Ludwig[3], Andreas Wieck[3], and Michael Oestreich[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung Nanostrukturen, Appelstr. 2, D-30167 Hannover, Germany — [2]Physikalisch Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany — [3]Ruhr-Universität Bochum, Angewandte Festkörperphysik, Universitätsstr. 150, D-44801 Bochum, Germany

We present new insights into single quantum dot (QD) spin noise spectroscopy (SNS) [1]. We have performed world's first measurements of

the single heavy hole spin dynamic in an individual (InGa)As QD by SNS [2]. These measurements reveal (a) very long T_1 hole spin lifetimes of up to 180 μs even in the low magnetic field range of up to 30 mT as well as (b) charge fluctuations in the QD surrounding. In order to suppress the parasitic influence of charge fluctuations, we move to QDs embedded in a Schottky diode structure which yields three main advantages: (i) the charge state of the QD, i.e., electron or hole, can be changed facilitating different coupling strength to the nuclear spin bath, (ii) the sharp single QD resonance can be tuned via the quantum confined Stark shift, and (iii) charge fluctuations are strongly reduced.

[1] J. Hübner, F. Berski, R. Dahbashi, and M. Oestreich, physica status solidi (b) **251**, 1824 (2014).

[2] R. Dahbashi, J. Hübner, F. Berski, K. Pierz, and M. Oestreich, Phys. Rev. Lett **112**, 156601 (2014).

TT 41.7 Tue 11:00 ER 270

Induced nuclear spin polarization in ZnSe:F epilayers — •Johan Erik Kirstein[1], Fabian Heisterkamp[1], Evgeny A. Zhukov[1], Alex Greilich[1], Dmitri R. Yakovlev[1,2], Irina A. Yugova[1,3], Vladimir L. Korenev[2], Alexander Pawlis[4], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Physical Faculty of St. Petersburg State University, 198504 St. Petersburg, Russia — [4]Department Physik, Universität Paderborn, 33098 Paderborn, Germany

We study the interaction of electron and nuclear spins in fluorine-doped ZnSe epilayers. Using the time-resolved optical pump-probe spectroscopy in the regime of resonant spin amplification we are able to resolve nuclear magnetic resonances (NMR) of ^{77}Se and ^{67}Zn isotopes with non-zero spin. The effective nuclear fields show a dispersive form of its strength around NMR as a function of magnetic field. In the RSA signal this leads a shift of the resonances of the electron spins. Dependences are measured as a function of external parameters, like: pump power, polarization modulation frequency and temperature. In a further experiment an external radio frequency field is applied to investigate the strength of the resulting nuclear field. Theoretical considerations support our findings.

TT 41.8 Tue 11:15 ER 270

Effect of electron spin inertia in II-VI semiconductors — •Fabian Heisterkamp[1], Evgeny A. Zhukov[1], Alex Greilich[1], Vladimir L. Korenev[1,2], Dmitri R. Yakovlev[1,2], Alexander Pawlis[3], Grzegorz Karczewski[4], Tomasz Wojtowicz[4], Jacek Kossut[4], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [4]Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland

An electron bound to a fluorine donor impurity in ZnSe has been considered as a good candidate for a quantum bit [1]. We study the spin relaxation time (T_1) in fluorine-doped ZnSe epilayers using optical pump-probe spectroscopy. We fix the time-delay between pump and probe pulse and scan the magnetic field in Faraday geometry to measure the polarization recovery curve for different pump helicity modulation frequencies. While the spin polarization is able to reach its steady-state value for low modulation frequencies, the spins cannot be polarized completely, if the pump helicity changes too fast. We present a theoretical model for this effect of electron spin inertia. To test this approach we determine the spin relaxation time also for resident electrons in CdTe QWs. For further information on the optical properties of the samples we refer to Refs. [2] and [3]. [1] Sanaka et al., Phys. Rev. Lett. 103, 053601 (2009). [2] Greilich et al., Phys. Rev. B 85, 121303(R) (2012). [3] Zhukov et al., Phys. Rev. B 76, 205310 (2007).

TT 42: Transport: Topological Insulators 3 (jointly with DS, HL, MA, O)

Time: Tuesday 14:00–16:00 Location: H 0110

TT 42.1 Tue 14:00 H 0110

Helical Surface States In Strained HgTe — •Jan Boettcher and Ewelina M. Hankiewicz — Universität Würzburg, Faculty for Physics and Astronomy, TP IV

Strained HgTe is a 3D topological insulator with negligible bulk conductivity, where the transport is dominated by the surface states for a wide density range [1]. We analytically show the existence of a topologically protected surface state within the framework of a simplified 6x6 Kane Hamiltonian defined on the half-space. Strained HgTe is different from other 3D TIs due to an additional coupling of the surface states, forming between the light-hole and electron-like (S) bands, to the heavy-hole bands. This coupling causes an avoided crossing between these bands and, therefore, opens a large gap in the surface state spectrum by which the topological protection is not affected. Furthermore, we investigate the spin texture of the surface states. In the presence of an external magnetic field, we study the Landau level spectrum and discuss the experimental signatures which would be a consequence of our model.

We acknowledge grant HA 5893/4-1 within SPP 1666.

[1] Brüne et al., arXiv:1407.6537 (to be published in PRX 2014).

TT 42.2 Tue 14:15 H 0110

Trasport signatures of a Zeeman-split quantum dot coupled to a helical edge state — •Benedikt Probst[1], Pauli Virtanen[2], and Patrik Recher[1] — [1]Institut für Mathematische Physik, TU Braunschweig, 38106 Braunschweig, Germany — [2]O.V. Lounasmaa Laboratory, Aalto University School of Science, Finland

We investigate the transport signatures of a Zeeman-split quantum dot (QD) containing a single spin 1/2 weakly coupled to a helical Luttinger liquid (HLL) within a generalized master equation approach. The HLL induces a tunable magnetization direction on the QD controlled by an applied bias voltage when the quantization axes of the QD and the HLL are noncollinear. This tunability allows to extract characteristic signatures of a HLL and the spin dynamics of the QD via the backscattering conductance and the current noise.

TT 42.3 Tue 14:30 H 0110

Effects of random Rashba spin-orbit coupling and magnetic impurities on edge state transport in topological insulators — Lukas Kimme[1], •Bernd Rosenow[1], and Arne Brataas[2] — [1]Institut für Theoretische Physik, Universität Leipzig, D-04103, Leipzig, Germany — [2]Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

CdTe/HgTe quantum-wells that exceed a critical thickness host topologically protected edge states, which give rise to a quantized conductance. Despite the topolgical protection, experimentally a mean free path of a few microns is found [1]. The experimentally observed weak temperature dependence of the mean free path challenges proposed theoretical explanations, many of which predict power law behaviors. We here consider a model where edge electrons experience spatially random Rashba spin-orbit coupling, and are also coupled to a magnetic impurity. Using a rate equation model, we determine the steady state of the impurity spin in the finite bias regime, and compute both linear and nonlinear resistances. For a finite density of impurity spins, we obtain a weak temperature dependence of the mean free path, in agreement with experimental findings.

[1] M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi, and S.-C. Zhang, Science 318, 766 (2007).

TT 42.4 Tue 14:45 H 0110

Spin-based Mach-Zehnder interferometry in topological insulator p-n junctions — •Fernando de Juan[1,2], Roni Ilan[1], and Joel E. Moore[1] — [1]University of California, Berkeley — [2]Freie Universität Berlin

A p-n junction, an interface between two regions of a material populated with carriers of opposite charge, is a basic building block of solid state electronic devices. From the fundamental physics perspective, it often serves as a tool to reveal the unconventional transport behavior of novel materials. In this work, we show that a p-n junction made from a three dimensional topological insulator (3DTI) in a magnetic field realizes an electronic Mach-Zehnder interferometer with virtually

perfect visibility. This is owed to the confinement of the topological Dirac fermion state to a closed two-dimensional surface, which offers the unprecedented possibility of utilizing external fields to design networks of chiral modes wrapping around the bulk in closed trajectories, without the need of complex constrictions or etching. Remarkably, this junction also acts as a spin filter, where the path of the particle is tied to the direction of spin propagation. It therefore constitutes a novel and highly tunable spintronic device where spin polarized input and output currents are naturally formed and could be accessed and manipulated separately.

TT 42.5 Tue 15:00 H 0110

Broken-gap topological insulators in magnetic fields — Rafał Skolasinski[1], Dimitry Pikulin[2], and •Michael Wimmer[1] — [1]Delft University of Technology, The Netherlands — [2]University of British Columbia, Canada

Two-dimensional topological insulators have helical edge channels protected by time-reversal symmetry, leading to a quantized conductance within the topological gap. A magnetic field breaks time-reversal symmetry, and thus is expected to break the quantization of conductance. Yet, recent experiments on topological insulators in broken-gap InAs/GaSb quantum wells have found very little dependence on magnetic field [1]. We discuss the effects of the orbital and the Zeeman part of the magnetic field on broken-gap quantum wells, and consider in which regime quantized conductance can be preserved.

[1] L. Du et al., arXiv:1306.1925

TT 42.6 Tue 15:15 H 0110

Cherenkov effect in topological insulators — •Sergey Smirnov — Institute for theoretical physics, Regensburg University, 93040 Regensburg, Germany

The Cherenkov radiation discovered experimentally by Cherenkov in optics of transparent media and theoretically explained later by Tamm and Frank reappears in solids where particles move faster than sound and, as a result, excite lattice vibrations or phonons. In both cases the photons or phonons are distributed within a forward cone centered around the momentum of the particle producing the Cherenkov light or sound.

Here we demonstrate that at high energies helical particles on surfaces of topological insulators excite anomalous Cherenkov sound outside the forward cone when the anisotropy of the surface states exceeds a critical value. The sound features many outstanding properties. In particular, at strong anisotropy it localizes into a few forward and backward beams propagating along specific directions [1].

At low energies we predict that an in-plane magnetic field applied to a surface of a topological insulator will asymmetrically reverse the Cherenkov sound. This asymmetric Cherenkov acoustic reverse may be of practical relevance in design of low energy electronic devices such as acoustic ratchets or, in general, in low power design of electronic circuits with an external control of the Cherenkov dissipation [2].

[1] S. Smirnov, Phys. Rev. B 88, 205301 (2013).
[2] S. Smirnov, Phys. Rev. B 90, 125305 (2014).

TT 42.7 Tue 15:30 H 0110

One-dimensional Dirac electrons on the surface of weak topological insulators — •Alexander Lau[1], Carmine Ortix[1], and Jeroen van den Brink[1,2] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [2]Department of Physics, TU Dresden, Germany

We show that a class of weak three-dimensional topological insulators feature one-dimensional Dirac electrons on their surfaces. Their hallmark is a line-like energy dispersion along certain directions of the surface Brillouin zone. Interestingly, these one-dimensional Dirac line degeneracies are topologically protected by a symmetry that we refer to as in-plane time-reversal invariance. As an example, we demonstrate how this invariance leads to Dirac lines in the surface spectrum of stacked Kane-Mele systems.

TT 42.8 Tue 15:45 H 0110

Fractional quantization of the topological charge pumped in a 1D superlattice — •Pasquale Marra[1], Roberta Citro[1,2], and Carmine Ortix[3] — [1]CNR-SPIN, I-84084 Fisciano (Salerno), Italy — [2]Dipartimento di Fisica "E. R. Caianiello", Universitá di Salerno, I-84084 Fisciano (Salerno), Italy — [3]Institute for Theoretical Solid State Physics, IFW Dresden, D-01069 Dresden, Germany

A one-dimensional quantum charge pump transfers a quantized charge in each pumping cycle. This quantization is topologically robust being analogous to the quantum Hall effect. The charge transferred in a fraction of the pumping period is instead generally not quantized. We show, however, that with specific symmetries in parameter space the charge transferred at well-defined fractions of the pumping period is quantized as integer fractions of the Chern number. We illustrate in details this fractional quantization in a one-dimensional Harper-Hofstadter model for both periodic and open boundary conditions, and discuss its relevance for cold atomic gases in optical superlattices.

[1] arxiv:1408.4457 [cond-mat]

TT 43: Superconductivity: Fe-based Superconductors – 122

Time: Tuesday 14:00–15:45 Location: H 2053

Topical Talk TT 43.1 Tue 14:00 H 2053

Magnetism and Superconductivity in Eu-Based Iron Pnictides — •Sina Zapf — 1. Physikalisches Institut, Universität Stuttgart, Germany

$EuFe_2As_2$ is an extraordinary parent compound of the iron pnictides, as it exhibits at low temperatures – additional to the Fe spin density wave – long-range magnetic order of the Eu^{2+} local moments. Nevertheless, bulk superconductivity around 30 K can be induced by mechanical pressure or chemical substitution.

In this talk we review the remarkable interplay of unconventional superconductivity, itinerant and local magnetism in Eu based iron pnictides. We focus on the appearance of a re-entrant spin glass phase that coexists with superconductivity [1] and an indirect magneto-elastic coupling, enabling the persistent magnetic detwinning by small magnetic fields [2].

This work was done in collaboration with the groups of D. N. Basov, R. Kremer, and P. Gegenwart.

[1] S. Zapf et al., Phys. Rev. Lett. 110, 237002 (2013)
[2] S. Zapf et al., Phys. Rev. Lett. 113, 227001 (2014)

TT 43.2 Tue 14:30 H 2053

Probing the density of states in $EuFe_{2-x}Ru_xAs_2$ — •Mamoun Hemmida[1], Hans-Albrecht Krug von Nidda[1], Axel Günther[1], Alois Loidl[1], Andreas Leithe-Jasper[2], Walter Schnelle[2], Helge Rosner[2], and Jörg Sichelschmidt[2] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Electron spin resonance of Eu^{2+} ($4f^7$, $S = 7/2$) in europium-based iron pnictides successfully probes the local density of states of the conduction electrons [1]. Starting from the mother compound $EuFe_2As_2$, the usual metallic phase is characterized by the linear increase of the linewidth on increasing temperature (Korringa slope $b = 8$ Oe K^{-1}) due to the Korringa relaxation via the conduction electrons, while this Relaxation contribution is switched off in the spin-density wave phase ($T < T_{SDW}$), where the linewidth is mainly determined by the crystal-electric field of the ligands [2]. Thus, we observe the same phenomenology like in insulators, despite of the high conductivity. Substitution of ruthenium for iron gradually suppresses the SDW phase up to $x = 0.5$ and reduces the Korringa slope down to about $b = 0.3$ Oe K^{-1} for $x = 2$. This indicates a continuously decreasing conduction-electron density of states at the Fermi energy on increasing Ru Substitution in a good agreement with band-structure calculations.

[1] M. Hemmida *et al.*, Phys. Rev. B **90**, 205105 (2014).
[2] E. Dengler *et al.*, Phys. Rev. B **81**, 024406 (2010).

TT 43.3 Tue 14:45 H 2053

Crystal growth and characterization of $SrFe_2(As_{1-x}P_x)_2$ — •Agnes Adamski, Fadoua Fouta, and Cornelius Krellner — Physikalisches Institut, Goethe Universität Frankfurt, D-60438 Frankfurt am Main, Germany

Among the various iron-arsenide-based superconductors, members of the AFe_2As_2 (A = Ba, Sr, Ca), the so called 122 family, have become model systems for exploring superconductivity in this new class of high-T_C superconductors. Recently it turned out, that the different substitution series result in very different temperature-concentration phase diagrams, especially in the region where antiferromagnetism disappears and superconductivity emerge. Furthermore, the symmetry of the superconducting order parameter tends to vary from one substitution series to another.

Here, we report on the optimization of the single crystal growth of $SrFe_2(As_{1-x}P_x)_2$ using the well-established self-flux technique. However, so far the exact melting temperatures of various flux to 122 compositions are not reported in the literature. We performed differential thermal analysis (DTA) to determine these melting points as function of flux to 122 ratio and for various phosphorous concentrations. Subsequently, the obtained samples were analyzed with electron microscope, energy dispersive x-ray analysis and powder diffractometry to determine the phase relations and distribution coefficients in this series.

TT 43.4 Tue 15:00 H 2053

Scanning Tunneling Spectroscopy of $SrFe_2(As_{1-x}P_x)_2$ — •Jasmin Jandke, Petra Wild, Michael Schackert, and Wulf Wulfhekel — Physikalisches Institut, Karlsruhe Institute of Technology, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Germany

The antiferromagnetic parent compound $SrFe_2As_2$ shows a supression of the spin density wave and a subsequent superconducting state upon partial substitution of As by P [1]. We investigated single crystals for four different P-concentrations x in the superconducting (x=0.35,0.46) as well as in the spin density wave phase (x=0,0.2). The superconducting samples display a v-shaped superconducting gap, which suggests nodal superconductivity in this system. Furthermore, we were able to determine the superconducting coherence length by measuring the spatial resolved superconducting density of states. From inelastic tunneling spectra it is possible to determine the Éliashberg function from the normal state [2]. We thus investigated bosonic excitations for the four different P-concentrations. Indeed, evidence suggests peaks which can be related to bosonic modes. The phonon an non-phonon mechanism for the origin of these peaks will be discussed.

[1] T. Kobayashi et al. *J.Phys.Soc.Jpn.* **81**, SB045 (2012)
[2] M. Schackert et al. arXiv:1402.0071 [con-3mat.supr-con]

TT 43.5 Tue 15:15 H 2053

Unusually high critical current of P-doped $BaFe_2As_2$ single crystalline thin film — •Fritz Kurth[1,2], Chiara Tarantini[3], Vadim Grinenko[1], Jens Hänisch[1,4], Jan Jaroszynski[3], Elke Reich[1], Yasohiro Mori[5], Akihiro Sakagami[5], Takahiko Kawaguchi[5], Jan Engelmann[1,2], Ludwig Schultz[1,2], Bernhard Holzapfel[4], Hiroshi Ikuta[5], Ruben Hühne[1], and Kazumasa Iida[1,5] — [1]IMW, IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]ASC, NHMFL, Florida, USA — [4]ITEP, KIT, Karlsruhe, Germany — [5]Department of Crystalline Materials Science, Nagoya University, Nagoya, Japan

Microstructurally clean, isovalently P-doped $BaFe_2As_2$ single crystalline thin films have been prepared by molecular beam epitaxy. These films show a superconducting transition temperature (T_c) of over 30 K and high transport self-field critical current densities (J_c) of over 6 MA/cm^2 at 4.2 K, which are among the highest for Fe based superconductors. In-field J_c exceeds 0.1 MA/cm^2 at $\mu_0 H = 35$ T for $H \| ab$ and $\mu_0 H = 18$ T for $H \| c$, respectively, in spite of moderate upper critical fields compared to other FeSCs with similar T_c. This unusually high J_c makes P-doped Ba-122 very favorable for high-field magnet applications.

TT 43.6 Tue 15:30 H 2053

Ultrafast structural dynamics of the Fe-pnictide parent compound $BaFe_2As_2$ — •L. Rettig[1], S.O. Mariager[1], A. Ferrer[1,2], S. Grübel[1], J.A. Johnson[1], J. Rittmann[1,3], T. Wolf[4], S.L. Johnson[2], G. Ingold[1], P. Beaud[1], and U. Staub[1] — [1]Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [2]ETH Zürich, CH-8093 Zürich, Switzerland — [3]EPFL, CH-1015 Lausanne, Switzerland — [4]KIT, D-76021 Karlsruhe, Germany

Understanding the interplay of the various degrees of freedom such as the electrons, spins and lattice is essential for many complex materials, including the high-temperature superconductors. In the Fe pnictides, especially the strong sensitivity of the electronic and magnetic properties to the Fe-As tetrahedra angle plays a crucial role for superconductivity and demonstrates a strong magneto-structural coupling.

Here, we use femtosecond time-resolved x-ray diffraction to investigate the structural dynamics in the Fe-pnictide parent compound $BaFe_2As_2$. We observe fluence dependent intensity oscillations of two specific Bragg reflections. Their distinctly different sensitivity to the pnictogen height demonstrates the coherent excitation of the A_{1g} phonon mode and allows us to quantify the coherent modifications of the Fe-As tetrahedra. By a comparison with time-resolved photoemission data we derive the electron-phonon deformation potential for this particular mode, which is comparable to theoretical predictions. Our results demonstrate the importance of this structural degree of freedom for the electron-phonon coupling in the Fe pnictides and indicate an ultrafast increase of the Fe magnetic moments.

TT 44: Correlated Electrons: Quantum-Critical Phenomena – Experiments

Time: Tuesday 14:00–15:45 Location: H 3005

TT 44.1 Tue 14:00 H 3005

Magnetic structure of $CeCu_2Ge_2$ and its implications on filed tuned quantum criticality — •Philipp Geselbracht[1], Karin Schmalzl[2], Micha Deppe[3], Christoph Geibel[3], and Astrid Schneidewind[4] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [2]Jülich Centre for Neutron Science (JCNS) at ILL, Forschungszentrum Jülich GmbH, Grenoble, France — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [4]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Garching, Germany

Recently, the common understanding of quantum criticality (QC) has been challenged for $CeCu_2Ge_2$ [1]. An external magnetic field can suppress the magnetic order, regardless of its direction, but only for the field along the a-direction, a quantum critical point could be identified. Such a behavior resembles the situation for QC of an Ising magnet in a transversal magnetic field, as already applied to less complicated model systems [2]. In this model, the field direction relative to the spin direction plays a crucial role. Therefore, we determined the magnetic structure of $CeCu_2Ge_2$ on a single crystal by means of polarized neutrons and solution of the magnetic structure. Our results are more thorough as in previous works [3], were the exact direction of the magnetic moments were left unclear. We will then interpret our new findings in analogy to the previous model systems.

[1] PRB 90, 155101 (2014).
[2] PRX 4, 031008 (2014).
[3] PRB 55, 6416-6420 (1997) and references.

TT 44.2 Tue 14:15 H 3005

Quantum Criticality in $Yb(Rh_{0.93}Co_{0.07})_2Si_2$ — •Alexander Steppke[1], Luis Pedrero[1,2], Robert Borth[1], Michael Nicklas[1], Cornelius Krellner[3], Christoph Geibel[1], Frank Steglich[1], and Manuel Brando[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Johann Wolfgang Goethe-Universität, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany

The heavy-fermion compound $YbRh_2Si_2$ is a prototype system which allows us to study an unconventional quantum critical point. With slight isoelectronic substitution of Rh by 7% Co the AFM order is stabilized ($T_N = 0.4$ K) and in thermodynamic ($\chi_{ac}(T)$) and electrical transport measurements ($\rho(T,H)$) the Kondo-breakdown energy scale T^* detaches from the putative conventional spin-density wave QCP [1]. To investigate the existence of this quantum phase transition and the possible role of the additional energy scale we performed thermodynamic measurements at low temperatures. At a QCP the absence of characteristic energy scales other than the temperatures has been shown to lead to power-law scaling behavior in the Grüneisen ratio

[2]. Combining results from specific heat, magnetization and thermal expansion we exclude a SDW QCP when the AFM order is suppressed by a magnetic field from the thermal and magnetic Grüneisen ratio. This is corroborated by measurements under hydrostatic pressure.

[1] S. Friedemann *et al.*, Nat. Phys. **5** (2009) 465.
[2] L. Zhu *et al.*, PRL **91** (2003) 066404.

TT 44.3 Tue 14:30 H 3005

Magnetic order in $CePd_{1-x}Ni_xAl$ — •Stefan Lucas[1], Zita Hüsges[1], Sarah Woitschach[1], Akito Sakai[2], Veronika Fritsch[2,3], Hilbert von Löhneysen[3], and Oliver Stockert[1] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]University of Augsburg, Augsburg, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

$CePd_{1-x}Ni_xAl$ is a heavy-fermion system, which shows both, geometric frustration arising from the hexagonal crystal structure and quantum critical behavior. By substituting palladium with nickel the Néel temperature of $T_N = 2.7$ K in CePdAl can be suppressed to zero at a nickel concentration of 14 %, where an antiferromagnetic quantum critical point is reached. Due to the combination of magnetic frustration and quantum criticality $CePd_{1-x}Ni_xAl$ may be a model system for investigating the influence of frustration on quantum critical behavior. To study the evolution of magnetic order in the substitution series detailed heat capacity measurements under magnetic fields were performed. The resulting phase diagrams for magnetic fields applied along the easy axis will be shown and discussed for CePdAl, the 5 %- and 10 %-nickel substituted system. A suppression of the Néel temperature as well as of the critical magnetic field are observed. In contrast to CePdAl no additional antiferromagnetic phases were detected in the Ni-alloyed systems. Furthermore, magnetic phase diagrams for fields applied along the hard ab-plane were established. Due to the frustration a slight increase of the ordering temperature was observed for small magnetic fields $B < 1$ T.

TT 44.4 Tue 14:45 H 3005

High-pressure Fermi surface of Mott insulator NiS_2 — •Sven Friedemann[1,2], Hui Chang[2], Monica Gamza[3], William Coniglio[4], David Graf[4], Stan Tozer[4], and F Malte Grosche[2] — [1]HH Wills Laboratory, University of Bristol, UK — [2]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [3]Department of Physics, Royal Holloway University of London, Egham, UK — [4]National High Magnetic Field Laboratory, Tallahassee, USA

Metals can turn into insulators when correlations become sufficiently strong. This is captured in the Mott-Hubbard model where onsite Coulomb repulsion leads to the opening of a gap at the Fermi energy for a half-filled band. This insulating state is realized for instance in the parent compounds of cuprate superconductors. Whilst cuprates are turned into metals by controlling the filling, i.e. doping, the metallic state can also be recovered by controlling the ratio of Coulomb repulsion and kinetic energy as can be done by pressure tuning. For this case, Luttinger theorem dictates the electrons to localize via a divergence of the effective mass [1]. Here, we report resistivity and quantum oscillation measurements on the pressure-induced insulator-to-metal transition in the Mott insulator NiS_2. We demonstrate the quality of our single crystals, discuss the phase diagram and present Fermi surface measurements in comparison with band structure calculations of the non-correlated case. We discuss these results in the light of the theoretical model.

[1] W. F. Brinkman, T. M. Rice; Phys Rev B; **10** 4302 (1970).

TT 44.5 Tue 15:00 H 3005

Neutron scattering of modulated magnetic order at the border of ferromagnetism in $NbFe_2$ — •Philipp G Niklowitz[1], Max Hirschberger[2], James Poulten[1], William Duncan[1], Andreas Neubauer[3], Petr Cermak[4], Astrid Schneidewind[4], Klaus Seemann[5], Enrico Faulhaber[5], Christian Pfleiderer[3], and F Malte Grosche[6] — [1]Dept of Physics, Royal Holloway, University of London, Egham, UK — [2]Dept of Physics, Princeton University, Princeton, USA — [3]Fakultät für Physik, TU München, Garching, Germany — [4]JCNS at MLZ, Forschungszentrum Jülich GmbH, Garching, Germany — [5]MLZ, TU München, Garching, Germany — [6]Cavendish Laboratory, University of Cambridge, Cambridge, UK

The border of ferromagnetism in the C14 Laves phase $NbFe_2$ is characterised by non-Fermi liquid properties consistent with ferromagnetic quantum criticality [1], but the ferromagnetic quantum critical point appears to be masked by modulated magnetic order (MMO).[2] With our elastic neutron scattering studies of three single-crystalline $Nb_{1-y}Fe_{2+y}$ samples ranging from Fe-rich composition to a nearly stoichiometric sample we have directly determined the ordering wave vector q_1 of MMO. A weak T and H and considerable y dependence of q_1 is observed. Our inelastic neutron data is dominated by strong quasielastic scattering in the vicinity of (002) and contains further features near q_1. The results indicate that $NbFe_2$ could display the theoretically predicted scenario of a ferromagnetic quantum critical point, which is masked by emerging modulated magnetic order.

[1] M. Brando *et al.*, PRL **101**, 026401 (2008).
[2] D. Rauch *et al.*, arXiv1312.2357

TT 44.6 Tue 15:15 H 3005

Effect of anisotropic strain on the quantum critical phase of $Sr_3Ru_2O_7$ — Daniel Brodsky[1,2], Mark Barber[1,2], •Clifford Hicks[1], Robin Perry[3], and Andrew Mackenzie[1,2] — [1]MPI-Chemische Physik fester Stoffe, Dresden, Germany — [2]Scottish Universities Physics Alliance (SUPA), School of Physics and Astronomy, University of St Andrews, St Andrews, UK — [3]SUPA, School of Physics, University of Edinburgh, Edinburgh, UK

We have developed a novel piezoelectric-based device for applying both compressive and tensile strains to single crystals. One particularly appealing target for such studies is $Sr_3Ru_2O_7$. $Sr_3Ru_2O_7$ has a novel quantum critical phase around a metamagnetic transition at 8 T, which shows very strong transport anisotropy in the presence of weak symmetry-breaking fields. We discuss the response of this phase to applied anisotropic lattice strain.

TT 44.7 Tue 15:30 H 3005

Towards ferromagnetic quantum criticality in $FeGa_{3-x}Ge_x$: ^{71}Ga NQR as a zero field microscopic probe — •Mayukh Majumder[1], Maik Wagner-Reetz[1], Raul Cardoso-Gil[1], Peter Gille[2], Yu Grin[1], and Michael Baenitz[1] — [1]Max Plank Institute for Chemical Physics of Solids, Dresden, Germany — [2]Ludwig-Maximilians-Universität Munchen, Germany

$FeGa_3$ is an ideal candidate to study the evolution of a metallic state and probably approaching to a ferromagnetic (FM) critical point upon Ge substitution by the local nuclear quadrupolar resonance (NQR) probe [1, 2]. ^{71}Ga NQR, magnetization and specific heat measurements have been performed in $FeGa_{3-x}Ge_x$ polycrystalline sample with x = 0.05, 0.1 (absent magnetic order), x = 0.15 (critical) and 0.2 ($T_C \sim 6$ K). NQR spectra provide direct information about the degree of local disorder (line width) and the critical fluctuations at the verge of FM ordering (spin-lattice relaxation at zero field). For x = 0.15 we found 3D quantum critical itinerant FM fluctuations and x = 0.2 exhibits weakly FM Moriya like behavior. Low doped samples surprisingly show heavy fermion behavior at low temperature ($\gamma = 70$ mJ/mole-K^2) with dominating antiferromagnetic correlations.

[1] Phys. Rev.B 86, 144421, (2012).
[2] arXiv: 1304.1897 (2013).
[3] Phys. Rev. B 89, 104426 (2014).

TT 45: Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 3 (jointly with DY)

Time: Tuesday 14:00–16:00 Location: H 3010

TT 45.1 Tue 14:00 H 3010

Real-time decay of a highly excited charge carrier in the one-dimensional Holstein model — •Florian Dorfner[1], Lev Vidmar[1], Christoph Brockt[2], Eric Jeckelmann[2], and Fabian Heidrich-Meisner[1] — [1]Ludwig-Maximilians-Universität München, Germany — [2]Leibniz Universität Hannover, Germany

We study the real-time dynamics of a highly excited charge carrier coupled to quantum phonons via a Holstein-type electron-phonon coupling [1]. This is a prototypical example for the non-equilibrium dynamics in an interacting many-body system where excess energy is transferred from electronic to phononic degrees of freedom. We use an efficient numerical method, i.e., diagonalization in a limited functional space, to study the non-equilibrium dynamics on a finite one-dimensional chain. We perform a comprehensive analysis of the time evolution in different parameter regimes by calculating the electron, phonon and electron-phonon coupling energies, and the electronic momentum distribution function. For example, we demonstrate that in the weak coupling regime, the relaxation dynamics obtained from the Boltzmann equation agrees very well with the numerical data. We also study the time dependence of the eigenstates of the single-site reduced density matrix, the so-called optimal phonon modes, unveiling that their structure in non-equilibrium contains very useful information for the interpretation of the numerical data. Support from the DFG through FOR 1807 is gratefully acknowledged.

[1] Dorfner et al, arXiv:1411.5074 (2014).

TT 45.2 Tue 14:15 H 3010

Measure of equilibration in Luttinger liquids — •Mariya Medvedyeva and Stefan Kehrein — Goettingen University, Goettingen, Germany

We consider the properties of the Luttinger liquid in the echo protocol (forward evolution in time followed by the backward evolution of slightly perturbed system) and explore the relation of the Loschmidt echo (the overlap of the initial and final wavefunctions) and the measurable properties of the system. We first study the linear Luttinger liquid as an example of an integrable system and find that the momentum distribution function exhibits almost complete recurrence while the Loschmidt echo does not, as the diagonal basis is different during the forward and backward time evolution. For a nonlinear Luttinger liquid the recurrence strength of the momentum distribution function drops as the nonlinearity of the fermion dispersion relation grows. We conclude that there is no simple relation of the Loschmidt echo to the behavior of the observables and that more work is needed to understand how to interpret the echo in the context of experiment.

TT 45.3 Tue 14:30 H 3010

Quantum Freezing Effect in 1D SU(N) Hubbard Systems — •Salvatore R. Manmana, Mariya V. Medvedyeva, and Johannes M. Oberreuter — Institut f. Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen

We investigate the time evolution of SU(N) Fermi-Hubbard systems by releasing initially trapped particles onto an empty lattice. Using the time-dependent DMRG and perturbative approaches, we find that in one spatial dimension for large enough filling and values of N, repulsive interactions cause the dynamics to develop a very strong freezing effect, i.e., on the time scales accessible, particle motion is essentially suppressed. We relate this finding to the quantum distillation effect previously reported for SU(2) Fermi-Hubbard systems and discuss its relevance for ongoing experiments with alkaline earth atom experiments on optical lattices.

TT 45.4 Tue 14:45 H 3010

Thermalization Dynamics in the Interacting Luttinger Model after a Quantum Quench — •Michael Buchhold and Sebastian Diehl — Institut für Theoretische Physik, TU Dresden, 01062 Dresden

Interacting Luttinger Liquids form a paradigmatic example of one-dimensional interacting fermions with a weak integrability breaking non-linearity. The thermalization dynamics of this model after an interaction quench is studied in a Keldysh non-equilibrium framework by means of Dyson-Schwinger equations.

After the quench, the ballistic dephasing of the phononic modes leads to correlations corresponding to a prethermal state, well described by a generalized Gibbs ensemble (GGE). This behavior is however overwritten on short distances by a sub-ballistically spreading thermal regime. While the GGE still features algebraic correlations in space and time with a corresponding non-equilibrium exponent, the thermal state shows the well-known exponential decay of correlations.

TT 45.5 Tue 15:00 H 3010

Spectral Properties of One-Dimensional Fermi Systems after an Interaction Quench — •Christian Klöckner, Dante Marvin Kennes, and Volker Meden — Institut für Theorie der Statistischen Physik, RWTH Aachen University and JARA - Fundamentals of Future Information Technology, 52056 Aachen, Germany

We show that the single-particle spectral properties of gapless one-dimensional Fermi systems in the Luttinger liquid state reached at intermediate times after an abrupt quench of the two-particle interaction are highly indicative of the unusual nonequilibrium nature of this state. Analytical and numerical insights gained by applying bosonization are presented. The resulting line shapes of the momentum-integrated and -resolved spectral functions strongly differing from their ground state as well as finite temperature equilibrium counterparts.

TT 45.6 Tue 15:15 H 3010

Inhomogeneous Quantum Quenches in the 1D Hubbard Model — •Ernst von Oelsen[1], Götz Seibold[1], and Jörg Bünemann[2] — [1]BTU Cottbus-Senftenberg — [2]Philipps-Universität Marburg

We investigate the dynamics of a many-electron system after a sudden quench of the single-particle potential and of the interaction strength. The calculation is based on the single-band Hubbard model and the time-dependent Gutzwiller theory. Our study is focussed on finite-size systems with lattice-site dependent on-site potentials and interaction strengths.

We compute the time-evolution of the electrons' density matrix and of the electrons double occupancy by fully integrating the equations of motion. Thus, our approach is not limited to small amplitudes but allows for a detailed study of the dependence of the electrons' excitation energies on both the interaction strength and the strength of the quench. Our results are compared to those from exact diagonalization techniques, from the small-amplitude limit and from a Hartree–Fock calculation.

TT 45.7 Tue 15:30 H 3010

Thermalization rates in a 1d Fermi-Hubbard model with slightly broken integrability for various fillings — •Fabian Biebl and Stefan Kehrein — Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany

Understanding relaxation in quantum systems is essential to determine whether an experimental setup can be described by equilibrium concepts. For example integrable systems do not thermalize, but develop into non-thermal steady states. By slightly breaking integrability, thermalization of such non-thermal (prethermalized) states becomes possible. An important question is to identify the corresponding timescale for thermalization due to the breaking of integrability.

We investigate this question for a fermionic Hubbard chain in the thermodynamic limit. The integrability breaking term is a small next to nearest neighbor hopping term [1,2]. The thermalization timescale is extracted from the quantum Boltzmann equation and depends strongly on temperature, especially when one goes away from half filling. The dependence on filling is connected to Umklapp-processes and we study this dependence systematically.

[1] M. L. R. Fuerst et al., Phys. Rev. E 86, 031122 (2012).
[2] M. L. R. Fuerst et al., Phys. Rev. E 88, 012108 (2013).

TT 45.8 Tue 15:45 H 3010

Time evolution of the ohmic spin boson model at finite bias in the weak coupling limit — •Carsten Lindner and Herbert Schoeller — Institut für Theorie der Statistischen Physik, RWTH Aachen

The spin boson model is a prominent model which describes dissipation in a quantum mechanical two-state system caused by an energy exchange with the environment. Proposed for applications in various fields of condensed matter physics, it has been discussed widely for more than twenty years. However, a full systematic analysis of the weak coupling regime has not been done for a long time. Recently, the time evolution of the ohmic spin boson model at zero bias has been investigated in the case of weak coupling where the interaction with the environment can be regarded as a small perturbation [1]. Therefore, a non-equilibrium renormalization group (RG) method, which has come to be known as the real-time RG (RTRG), has been employed to determine its time evolution. The choosen approach allows to obtain the time evolution in a controlled way which means that the renormalized coupling parameters stay small for arbitrarily long times. Beside predicting the dominant exponential time evolution, this method also enables us to address the time scaling behavior of the pre-exponential functions precisely. Based on this insight, we have investigated the ohmic spin boson model at finite bias accordingly, leading to new results on all time scales.

[1] O. Kashuba and H. Schoeller, Phys. Rev. B 87, 201402(R) (2013)

TT 46: Transport: Nanomechanics (jointly with MM)

Time: Tuesday 14:00–15:45 Location: A 053

TT 46.1 Tue 14:00 A 053

Inductively coupled cavity optomechanics — •P. Schmidt[1,2], M. Pernpeintner[1,2,3], K.F. Wulschner[1,2], S.T.B. Goennenwein[1,3], A. Marx[1], R. Gross[1,2,3], and H. Huebl[1,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Nanosystems Initiative Munich, München, Germany

Cavity optomechanics allows to study the light-matter interaction with micro-, meso-, and macroscopic objects offering the possibility to access the quantum mechanical regime in the literal sense [1]. Transferring this approach to the microwave (MW) domain gives rise to the field of cavity electromechanics. Typical electromechanical systems consist of a micro- or nanomechanical resonator coupled capacitively to a superconducting MW resonator.
Here, we present the approach of an inductively coupled electromechanical system. To this end, we implement a dc-SQUID with a vibrational element at the current antinode of a $\lambda/4$ MW resonator. Hereby, the eigenfrequency of the MW resonator becomes tunable. As the vibration of the nano-string changes the SQUID loop area, we expect that the electromechanical coupling becomes flux-tunable.
We present first experimental results obtained from MW transmission spectroscopy in a dilution refrigerator and compare it with our theoretical model. These results indicate an expected tunability of the electromechanical coupling from 0 to 1 kHz.

[1] M. Aspelmeyer *et al.*, Physics Today **65**, 29 (2012).

TT 46.2 Tue 14:15 A 053

Circuit Electromechanics with a Non-Metallized Nanobeam — •Matthias Pernpeintner[1,2,3], T. Faust[4], F. Hocke[1,2,3], J. P. Kotthaus[4], E. M. Weig[4,5], R. Gross[1,2,3], and H. Huebl[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Nanosystems Initiative Munich, München, Germany — [3]Physik-Department, Technische Universität München, Garching, Germany — [4]Center for NanoScience (CeNS) and Fakultät für Physik, Ludwig-Maximilians-Universität, München, Germany — [5]Department of Physics, University of Konstanz, Konstanz, Germany

In the field of cavity optomechanics, a motional degree of freedom is coupled to an optical cavity. This approach can be transferred to the solid state environment e. g. by combining a superconducting microwave cavity with a nanomechanical resonator.

Whereas typically metallized mechanical resonators are used, we present an alternative approach which is based on the dielectric coupling between a superconducting coplanar waveguide microwave resonator and a non-metallized tensile-stressed silicon nitride nanobeam.

We use the Duffing nonlinearity of the strongly driven beam to calibrate the amplitude spectrum of the mechanical motion and determine the electromechanical vacuum coupling. We find a quality factor of 480,000 at a resonance frequency of 14 MHz and 0.5 K. We deduce a vacuum coupling of 11.5 mHz, which is in quantitative agreement with finite element based model calculations.

This type of hybrid platform will allow further studies on the properties of non-metallized beams and more complex mechanical hybrids.

TT 46.3 Tue 14:30 A 053

Coupling Graphene Mechanical Resonators to Superconducting Microwave Cavities — •Peter Weber, Johannes Güttinger, Ioannis Tsioutsios, Darrick E. Chang, and Adrian Bachtold — ICFO-Institut de Ciencies Fotoniques, 08660 Castelldefels (Barcelona), Spain

Graphene is an attractive material for nanomechanical devices because it allows for exceptional properties, such as high frequencies, quality factors, and low mass. An outstanding challenge, however, has been to obtain large coupling between the motion and external systems for efficient readout and manipulation. Here, we report on a novel approach, in which we capacitively couple a high-Q graphene mechanical resonator (Q = 100.000) to a superconducting microwave cavity. The initial devices exhibit a large single-photon coupling of ˜10 Hz. Remarkably, we can electrostatically change the graphene equilibrium position and thereby tune the single photon coupling and the mechanical resonance frequency by a large amount. The strong tunability opens up new possibilities, such as the tuning of the optomechanical coupling strength on a time scale faster than the inverse of the cavity line width. With realistic improvements, it should be possible to enter the regime of quantum optomechanics.

TT 46.4 Tue 14:45 A 053

Spin-vibration interaction in a nanomechanical spin-valve — •Pascal Stadler[1], Wolfgang Belzig[1], and Gianluca Rastelli[1,2] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Zukunftskolleg, Fachbereich Physik, Universität Konstanz, 78457, Konstanz, Germany

We study spin-dependent transport in a suspended carbon nanotube quantum dot in contact with two ferromagnetic leads and with the dot's spin interacting with the flexural modes [1,2]. The spin-vibration interaction arises from the spin-orbit coupling or a magnetic field gradient. We use a nonequilibrium Green's functions technique to evaluate the phonon occupation and the transport properties. The interaction between the spin and the vibration leads to a mechanical damping and, for an applied bias-voltage, to a steady nonequilibrium occupation of the harmonic oscillator. Depending on the magnetic configuration and the bias voltage polarity, a single vibrational mode can be strongly cooled, heated or can approach a regime of a mechanical instability. Owing to the sensitivity of the electron transport to the spin orientation, we find signatures of the nanomechanical motion in the current-voltage characteristic.

[1] P. Stadler, W. Belzig, and G. Rastelli,
Phys. Rev. Lett. **113**, 047201 (2014).
[2] P. Stadler, W. Belzig, and G. Rastelli, arXiv:1408:6357.

TT 46.5 Tue 15:00 A 053

Large current noise in nanoelectromechanical systems close to continuous mechanical instabilities — Jochen Brüggemann[1], •Guillaume Weick[2], Fabio Pistolesi[3], and Felix von Oppen[4] — [1]I. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany — [2]Institut de Physique et Chimie des Materiaux de Strasbourg, Université de Strasbourg, CNRS UMR 7504, F-67034 Strasbourg, France — [3]Laboratoire Ondes et Matiere dÁquitaine, Université de Bordeaux, CNRS UMR 5798, F-33400 Talence, France — [4]Dahlem Center for Complex Quantum Systems & Fachbereich Physik, Freie Universität Berlin, D-14195 Berlin, Germany

We investigate the current noise of nanoelectromechanical systems close to a continuous mechanical instability. In the vicinity of the latter, the vibrational frequency of the nanomechanical system vanishes, rendering the system very sensitive to charge fluctuations and, hence, resulting in very large (super-Poissonian) current noise. Specifically, we consider a suspended single-electron transistor close to the Euler buckling instability [1,2,3]. We show that such a system exhibits an

exponential enhancement of the current noise when approaching the Euler instability which we explain in terms of telegraph noise [4].

[1] G. Weick et al., PRB 81, 121409(R) (2010)
[2] G. Weick et al., PRB 83, 035420 (2011)
[3] G. Weick et al., PRB 84, 125454 (2011)
[4] J. Brüggemann et al., PRB 85, 125441 (2012)

TT 46.6 Tue 15:15 A 053

Mechanically induced iSWAP gate and maximally entangled states in a carbon nanotube — •Heng Wang and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We study a nanomechanical system where two separated single-electron spins in two quantum dots in a suspended carbon nanotube (CNT) are driven by an ac electric field in a parallel magnetic field. An indirect coupling between two single-electron spins is induced based on the simultaneous interaction of the two spins with the mechanical mode of the CNT. We show how a two-qubit iSWAP gate and arbitrary single-qubit gate can be obtained by analyzing the effective Hamiltonian from the time dependent Schrieffer-Wolff transformation and the time evolution operator. Combining the iSWAP gate and single-qubit gates, maximally entangled states of two spins can be generated with a single step by varying the frequency and the strength of the external electric driving field. The iSWAP gate and single-qubit gates can be turned off when suppressing the spin-phonon coupling by electrostatically shifting the electron wave function on the nanotube.

TT 46.7 Tue 15:30 A 053

Nonlinear phononics using atomically thin membranes — Daniel Midtvedt and •Alexander Croy — Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany

In recent years, there has been considerable interest in tailoring material and wave-propagation properties using structured materials, prominent examples being phononic and photonic crystals. Here, we propose a design that allows for engineering flexural-phonon propagation by facilitating atomically thin membranes [1]. The strong geometric nonlinearity present in such systems leads to phonon-phonon interactions, which allow the study of many-body effects. Using a continuum mechanics description of a periodically pinned graphene membrane, we investigate the properties of the resulting phononic crystal and demonstrate that defects in the pinning lattice support localized modes. Two such modes in close proximity interact via the elastic energy, and constitute a simple model of a phononic dimer. We show that the defect Hamiltonian in the rotating-wave approximation is equivalent to a classical Bose-Hubbard model. By tuning the properties of the pinning lattice and the amplitudes of the flexural vibrations, we observe a bifurcation corresponding to the transition from "Rabi" to "Josephson" dynamics. Further, we demonstrate a wide tunability of the dimer frequencies by local back-gates, which allows for studies of the (non-linear) Landau-Zener transition.

[1] D. Midtvedt, A. Isacsson and A. Croy, Nat. Commun. **5**, 4838 (2014).

TT 47: Organic Electronics and Photovoltaics: OPV I (jointly with CPP, HL, O)

Time: Tuesday 14:00–16:00 Location: C 130

Invited Talk TT 47.1 Tue 14:00 C 130

Ultrafast Coherent Charge Transfer in Solar Cells and Artificial Light Harvesting Systems — •Christoph Lienau[1], Ephraim Sommer[1], Antonietta de Sio[1], Ralf Vogelgesang[1], Margherita Maiuri[2], Giulio Cerullo[2], Angel Rubio[3], Carlo A. Rozzi[4], and Elisa Molinari[4] — [1]Carl von Ossietzky University, Oldenburg, Germany — [2]Politecnico di Milano, Milano, Italy — [3]Universidad del País Vasco, San Sebastian, Spain — [4]Dipartimento di Scienze Fisiche, Modena, Italy

To elucidate the fundamental microscopic processes in solar energy conversion, we have recently combined coherent femtosecond spectroscopy and first-principles quantum dynamics simulations [1,2] and have used this approach to explore the primary photoinduced electronic charge transfer in two prototypical structures: (i) a carotene-porphyrin-fullerene triad, an elementary component for an artificial light harvesting system [2] and (ii) a polymer:fullerene blend as a model for an organic solar cell [1].

Our results provide strong evidence that in both systems, at room temperature, the driving mechanism of the primary step within the current generation cycle is a quantum-correlated wavelike motion of electrons and nuclei on a timescale of few tens of femtoseconds. They suggest that the strong coupling between electronic and vibrational degrees of freedom is of key importance for the dynamics and yield of the charge separation process. Here, I will discuss our most recent experimental and theoretical findings. [1] S. M. Falke et al., Science 344, 6187 (2014). [2] C. A. Rozzi et al., Nature Comm. 4, 1602 (2013)

TT 47.2 Tue 14:30 C 130

Calculation of exciton dissociation rates in ordered and disordered 2D model organic photovoltaic interfaces — •Hector Vazquez[1] and Alessandro Troisi[2] — [1]Inst. of Physics, Academy of Sciences of the Czech Rep., CZ — [2]Dept. of Chemistry and Centre of Scientific Computing, University of Warwick, UK

The efficient generation of free charges from incident light in organic photovoltaic cells has been studied extensively but is not yet well understood. In order to separate, electron and hole have to overcome the Coulomb attraction and several mechanisms have been proposed. In particular, 'hot' excitons having excess energy have received a lot of attention but no consensus yet exists [1].

In this talk, I will introduce a method to calculate exciton dissociation rates [2] and will describe its application to 2-Dimensional model organic photovoltaic interfaces. The method uses Green's functions within a widely applicable model Hamiltonian of donor/acceptor interfaces with and without disorder. Initial states are Frenkel excitons while final states are Charge-Transfer (CT) states. I will present results for the generation rates of CT states where I will highlight the importance of disorder and the delocalization of the excitonic wavefunctions. Excitons dissociate into 'hot' CT states with partially separated charges, where electron and hole are located far from the interface.

1) A. A. Bakulin et al., Science 335, 1340 (2012), A. E. Jailaubekov et al., Nat. Mater. 12 66 (2013), G. Grancini et al., Nat. Mater. 12 29 (2013), K. Vandewal et al., Nat. Mater. 13 63 (2013).
2) H. Vazquez, A. Troisi, Phys. Rev. B 88, 205304 (2013).

TT 47.3 Tue 14:45 C 130

Charge separation at C_{60}/P3HT and P3HT/ZnO interfaces probed by femtosecond time-resolved second harmonic generation measurements — •Marc Hänsel[1], Michael Schulze[1], Yunus Sevinchan[2], Yana Vaynzof[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Heidelberg, Germany — [2]Centre of Advanced Materials, Heidelberg, Germany

A deeper understanding of the process of ultrafast charge transfer and separation at donor/acceptor interfaces is a prerequisite for improvement of organic and hybrid solar cells. Time-resolved second harmonic generation (TR-SHG) with femtosecond temporal resolution was used to investigate different donor/acceptor interfaces. With this intrinsically interface sensitive technique we were able to monitor the charge transfer dynamics of the well-defined single heterojunctions C_{60}/P3HT and P3HT/ZnO. In addition some modifications via cesium doping were made to the ZnO/P3HT interface. At the C_{60}/P3HT interface a pump energy dependent ultrafast charge transfer state with a population time of 320fs has been observed.

TT 47.4 Tue 15:00 C 130

Modelling charge transfer in Polymer/SWNT/PCMB hybrid systems — •Livia Glanzmann, Duncan Mowbray, and Angel Rubio — Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Universidad del Pais Vasco UPV/EHU, Av. Tolosa 72, E-20018 San Sebastian, Spain

One way to increase power conversion efficiencies of organic photovoltaic devices (OPVs) is to optimize the electron donor (D) acceptor (A) materials. The level alignment of the frontier orbitals at the D-A heterojunction interface is important for an efficient charge transfer. Since the first heterojunction OPV, consisting of 3-alkylpolythiophene (P3HT) and Fullerene, several combinations of D-A materials were tested. As well, carbon nanotubes were introduced, which increased

the efficiency of such multi-component systems. Still, the electronic processes within such systems are not well understood. To shed light on this subject, we simulate photovoltaic processes occuring in selected sets of P3HT-based-Polymer/SWNT or PCBM heterojunctions. As a first step, we create the excited states within the donor materials by performing TDDFT calculations and extract the electron density of the exciton. Then, we use the delta SCF approach to study the D-A electron transfer. On top, we calculate the probability of an electron passing the D-A interface and being transported through a nanotube by performing G0W0 calculations. All these results show the effect of certain types of D-A material, as well of their level alignment, on the efficiency of OPVs.

TT 47.5 Tue 15:15 C 130

Photoinduced Dynamics of Charge Separation: from Photosynthesis to Polymer-Fullerene Bulk-Heterojunctions — •Andreas Sperlich[1], Oleg G. Poluektov[2], Jens Niklas[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Chemical Sciences and Engineering Division, ANL, Argonne, Illinois 60439, USA — [3]ZAE Bayern, 97074 Würzburg

Understanding charge separation and charge transport is crucial for improving the efficiency of organic solar cells. This is due to the excitonic nature of their active media, based on organic molecules, serving as both a light absorbing and transport layer. Charge transfer (CT) states play an important role, being intermediate for free carrier generation and charge recombination. Here, we use light-induced electron paramagnetic resonance (EPR) spectroscopy to study the charge transfer dynamics in composites of the polymers P3HT, PCDTBT, and PTB7 with the fullerene derivative $PC_{60}BM$. Transient EPR measurements show strong spin-polarization patterns for all polymer-fullerene blends, confirming predominant generation of singlet CT states. These observations allow a comparison with charge separation processes in molecular donor-acceptor systems, as found in natural and artificial molecular photosynthetic systems and clarification of the initial steps of sequential charge transfer in organic photovoltaic (OPV) materials. The detection of strong electron spin-polarization in OPV materials points out to the significance of spin dynamics for the efficient functioning of solar cell devices.

TT 47.6 Tue 15:30 C 130

Sub-ns Triplet State Formation in PSBTBT:PC70BM and PCPDTBT:PC60BM Photovoltaic Blends — Fabian Etzold[1], Ian Howard[1,2], and •Frédéric Laquai[1] — [1]Max Planck Research Group for Organic Optoelectronics, Max Planck Institute for Polymer Research, D-55128 Mainz, Germany — [2]Institute of Microstructure Technology (IMT), Karlsruhe Institute of Technology (KIT), D-76344 Eggenstein-Leopoldshafen, Germany

The excited state dynamics in low-bandgap polymer:fullerene blends using the donor-acceptor copolymers PCPDTBT and its silicon-substituted analogue PSBTBT are investigated by femto- to microsecond broadband Vis-NIR transient absorption (TA) pump-probe spectroscopy. The TA experiments and analysis of the TA data by multivariate curve resolution (MCR-ALS) reveal that after exciton dissociation and free charge formation is completed, fast sub-nanosecond nongeminate recombination occurs and leads to a substantial population of the polymer's triplet state. The extent to which triplet states are formed depends on the initial concentration of free charges, which itself is controlled by the microstructure of the blend, especially in case of PCPDTBT:PC60BM. Interestingly, PSBTBT:PC70BM blends show a higher charge generation efficiency, but less triplet state formation at similar free charge carrier concentrations. This indicates that the solid-state morphology and interfacial structure of PSBTBT:PC70BM blends reduce non-geminate recombination and thus triplet state formation, leading to increased device performance compared to optimized PCPDTBT:PC60BM blends.

TT 47.7 Tue 15:45 C 130

Triplet Exciton Formation in High-Efficiency Donor-Acceptor Photovoltaic Blends — •Stefan Väth[1], Hannes Kraus[1], Andreas Baumann[2], Kristofer Tvingstedt[1], Andreas Sperlich[1], Vladimir Dyakonov[1,2], John Love[3], and Thuc-Quyen Nguyen[3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg — [3]University of Santa Barbara, Santa Barbara, CA 93106, USA

In donor-acceptor based bulk-heterojunction solar cells, the splitting of singlet excitons at the donor and acceptor interface is of crucial importance for charge generation. The reversed process, in which two initially free charge carriers meet at the interface to form an exciton with singlet or triplet multiplicity is rather beneficial for light emission in OLEDs but considered as one of the loss factors in OPV.

In our experiments, the occurrence of triplet excitons and CT states was probed by using spin sensitive detection of the photo- and electroluminescence. A substantial generation of molecular triplet excitons was found in high efficiency donor-acceptor OPV systems based on the low bandgap copolymer PTB7 and in the soluble small molecule p-DTS(FBTTh2)2, both blended with PC70BM as acceptor. We ascribe these findings to an electron back transfer from the CT state to the triplet state on the donor material. In summary, the fundamental understanding of the transformation processes involving the CT states, triplet excitons, as well as free electrons and holes and their dependence on nanoscale morphology and energetics of blends is essential for the optimization of OPV devices.

TT 48: Quantum Chaos (jointly with DY)

Time: Tuesday 14:30–16:00 Location: BH-N 334

TT 48.1 Tue 14:30 BH-N 334

Regular phase-space structures and bifurcations in generic 4D symplectic maps — •Franziska Onken[1], Steffen Lange[1], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

The dynamics of Hamiltonian systems (e.g., planetary motion, electron dynamics in nano-structures, molecular dynamics) can be investigated by symplectic maps. While a lot of work has been done for 2D maps, much less is known for higher dimensions.

For a generic 4D map regular 2D-tori are organized around a skeleton of families of elliptic 1D-tori [1], which can be visualized by 3D phase-space slices [2]. We present an analysis of the different bifurcations of the families of 1D-tori in phase space and in frequency space by computing the involved hyperbolic and elliptic 1D-tori. Applying known results of normal form analysis, both the local and the global structure can be understood: Close to a bifurcation of a 1D-torus, the phase-space structures are surprisingly similar to bifurcations of periodic orbits in 2D maps. Far away the phase-space structures can be explained by remnants of broken resonant 2D-tori.

[1] S. Lange, M. Richter, F. Onken, A. Bäcker and R. Ketzmerick, *Global structure of regular tori in a generic 4D symplectic map*, Chaos **24**, 024409 (2014)

[2] M. Richter, S. Lange, A. Bäcker, and R. Ketzmerick, *Visualization and comparison of classical structures and quantum states of four-dimensional maps*, Phys. Rev. E **89**, 022902 (2014)

TT 48.2 Tue 14:45 BH-N 334

How to deform a dielectric microcavity to get a given emission directionality — •Marcus Kraft and Jan Wiersig — Otto-von-Guericke-Universität Magdeburg, 39016 Magdeburg

An important characteristic of dielectric microcavities is the far field emission pattern. Here, we present a method to find an optimized deformation of the boundary of a microcavity to get a predetermined far field pattern. We write the symmetric deformation of the boundary in a Fourier series and put this ansatz into a perturbation theory for weakly deformed microcavities. By minimizing the difference between the resulted and desired far field pattern we develop a system of linear equations for the Fourier coefficients of the deformed boundary. A comparison to full numerical calculations is also presented.

TT 48.3 Tue 15:00 BH-N 334

Quantum Ergodicity in Open Chaotic Systems? — •Konstantin Clauss[1], Martin Körber[1], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]TU Dresden, Institut für Theoretische Physik, Dresden — [2]MPI für Physik komplexer Systeme, Dresden

In open quantum systems a fundamental question concerns the phase-space localization of resonance states. For a fully chaotic phase space the resonance states are supported on a fractal set of classically trapped orbits. We investigate the possibility of quantum ergodicity, i.e. semiclassical equidistribution with respect to suitable classical densities on this fractal set. We explain why these classical densities have to be chosen according to the quantum decay rate.

TT 48.4 Tue 15:15 BH-N 334

Frobenius-Perron operator for asymmetric backscattering in deformed microdisk cavities — •Julius Kullig and Jan Wiersig — Institut für Theoretische Physik, Universität Magdeburg, Germany

Due to radiation and absorption optical microcavities cannot be described by hermitian but non-hermitian Hamiltonians of open quantum systems. This leads in general to non-orthogonal quasibound states. In case of asymmetric optical cavities this is related to an imbalance between clockwise (CW) and counter-clockwise (CCW) propagating waves which manifests in a finite chirality of quasibound states [1, 2, 3, 4]. This has applications e.g. in optical sensors [5], where so-called exceptional points in parameter space can be used to enhance sensitivity [6].

We study the backscattering process between CW and CCW waves from pure classical ray dynamics. To this end we construct a finite approximation of Frobenius-Perron operator $\mathcal{F}$ to describe the time evolution of phase-space densities. The eigenstates of $\mathcal{F}$ show interesting analogues to quasibound states, including non-orthogonality and chirality. Our method is demonstrated for a spiral geometry and the asymmetric Limaçon.

[1] J. Wiersig, S. W. Kim and M. Hentschel PRA 78, 053809 (2008); [2] J. Wiersig, A. Eberspächer, J.-B. Shim, J.-W. Ryu, S. Shinohara, M. Hentschel and H. Schomerus PRA 84, 023845 (2011); [3] J. Wiersig PRA 84, 063828 (2011); [4] J. Wiersig PRA 89, 012119 (2014); [5] F. Vollmer, L. Yang, Nanophotonics 1, 267 (2012); [6] J. Wiersig PRL 112, 203901 (2014)

TT 48.5 Tue 15:30 BH-N 334

Ray-path reversal and Loschmidt echo for light beams — •Pia Stockschläder and Martina Hentschel — Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

A fundamental feature in classical geometrical optics is the reversibility of the light path. In reality, however, all light beams have finite width in contrast to the geometrical rays. This leads to corrections to ray optics – beam shift effects known as Goos-Hänchen shift and Fresnel filtering – which break ray-path reversibility. Here, we investigate in detail the influence of these corrections on the reversal of the optical path for a light beam reflected at a dielectric interface. As a measure of how much the reversed light path differs from the original one, we define and calculate a Loschmidt echo-like quantity in this context. As a possible technical application, we discuss the potential utilization of broken ray-path reversibility in optical sensors.

TT 48.6 Tue 15:45 BH-N 334

Quantum-classical correspondence in electronic transport through quantum point contacts — •Kazuhiro Kubo and Martina Hentschel — Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

We investigate the propagation of electrons starting from a quantum point contact like source in a random potential. We present the density of classical trajectories which clearly shows the well-known branching pattern near the source and its gradual disappearance at larger distances. We calculate the semiclassical Green's function for each trajectory, and discuss how its amplitude is related to both the branching features and the conjugate points (caustics) along the trajectory. Furthermore, we complement these discussions by including quantum mechanical results.

TT 49: Frontiers of Electronic Structure Theory: Charge and Spin Dynamics (jointly with O, HL)

Time: Tuesday 14:00–15:45 Location: MA 004

Invited Talk TT 49.1 Tue 14:00 MA 004

First-principles theories of electron-plasmon and electron-spin fluctuation interactions in nanomaterials — •Johannes Lischner — Imperial College, London, United Kingdom

The GW method includes an accurate treatment of many-electron interaction effects beyond density-functional theory and is the state-of-the-art approach for computing spectral functions and quasiparticle energies in nanomaterials. These quantities are measured in photoemission and tunneling experiments. Despite its great success, the GW approach has certain shortcomings and I will discuss two topics that require going beyond GW: i) plasmon satellites in spectral functions and ii) the coupling of quasiparticles to spin fluctuations.

Plasmon satellites in recent photoemission experiments on doped graphene have been interpreted in terms of novel plasmaron excitations, strongly coupled plasmon-hole states, predicted by GW theory. Using a cumulant expansion of the Green's function to include higher-order electron-electron interaction effects and an accurate description of the substrate, I will demonstrate that no plasmaron states need to be invoked to explain the experiments. Similar conclusions are drawn for tunneling spectra of semiconductor quantum-well two-dimensional electron gases. I will also discuss the interaction of quasiparticles with spin fluctuations in iron selenide and demonstrate that significant coupling constants can give rise to superconducting transition temperatures consistent with experimental findings.

TT 49.2 Tue 14:30 MA 004

Charge separation dynamics and opto-electronic properties of a diaminoterephthalate-C60 dyad — •Stefano Pittalis[1], Alain Delgado[1], Jörg Robin[2], Lena Freimuth[3], Jens Christoffers[3], Christoph Lienaua[2], and Carlo Andrea Rozzi[1] — [1]Istituto Nanoscienze - CNR, Modena, Italy — [2]Institut fuer Physik and Center of Interface Science, Carl von Ossietzky Universität, Oldenburg, Germany — [3]Institut fuer Chemie and Center of Interface Science, Carl von Ossietzky Universität, Oldenburg, Germany

A novel dyad composed of a diaminoterephthalate scaffold, covalently linked to a Fullerene derivative, is explored as a nanosized charge separation unit powered by solar energy. Its opto-electronic properties are studied and the charge separation rate is determined. Simulations of the coupled electronic and nuclear dynamics in the Ehrenfest approximation are carried out on a sub 100 fs time scale after photoexcitation in order to gain insights about the mechanisms driving the the charge separation. In particular, the role of vibronic coupling and of the detailed morphology are highlighted.

TT 49.3 Tue 14:45 MA 004

Transfering spin into an extended π-orbital of a large molecule – ab-initio study of Au-PTCDA:Au(111) — •T. Deilmann[1], T. Esat[2], B. Lechtenberg[3], P. Krüger[1], C. Wagner[2], R. Temirov[2], F.B. Anders[3], F.S. Tautz[2], and M. Rohlfing[1] — [1]Institut für Festkörpertheorie, Universität Münster, Germany — [2]Peter Grünberg Institute (PGI-3), FZ Jülich, Germany — [3]Lehrstuhl für Theoretische Physik II, TU Dortmund, Germany

The combination of an organic molecule with an unpaired spin offers a large variety of interplay between spins and orbitals, with high sensitivity to structural and environmental details. Recently, a single Au atom on a PTCDA monolayer physisorbed on Au(111) has been investigated experimentally; it exhibits a Kondo peak in the STS spectrum.

In this talk we discuss ab-initio mean-field electronic spectra (which will then serve as input data for a subsequent NRG calculation to describe the Kondo effect). Based on ab-initio structural data (in agreement with observed STM images) we evaluate the electronic spectra by many-body perturbation theory within the *GW* approximation, as well as, a simplified LDA+*GdW* approach [1]. For gas-phase PTCDA and Au-PTCDA, both methods agree well with one another and with available measurements. For Au-PTCDA on Au(111), a full *GW* calculation is too expensive due to the substrate. LDA+*GdW*, on the other hand, fully allows to incorporate the substrate polarizability in the self energy inside the molecule and leads to good agreement with the experimental data.

[1] M. Rohlfing, *Phys. Rev. B* **82**, 205127 (2010).

TT 49.4 Tue 15:00 MA 004

Quasi-particle band structure of the transition-metal-based zero-gap semiconductors — •Murat Tas[1], Ersoy Sasioglu[2], Iosif Galanakis[3], Christoph Friedrich[2], and Stefan Blügel[2] — [1]Department of Basic Sciences, İstanbul Kemerburgaz University, 34217 İstanbul, Turkey — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [3]Department of Materials Science, School of Natural Sciences, University of Patras, GR-26504 Patra, Greece

Zero-gap semiconductors (SCs) are promising materials for a variety of applications ranging from spintronics to thermoelectricity. Using the *GW* approximation within the framework of the FLAPW method, we study the quasi-particle band structure of a number of transition-metal-based zero-gap SCs XX′YZ, where X, X′ and Y are the transition metal elements, and Z is an *sp* element. We find that, in contrast to *sp*-electron based SCs such as Si and GaAs, the many-body renormalization has a minimal effect on the electronic band structure of these systems. It turns out that for many compounds the change of the band gap is less than 0.2 eV, which makes the starting point PBE a good approximation for the description of the electronic properties of these materials. Furthermore, the band gap can be tuned either by the variation of the lattice parameter or by the substitution of the Z element.

TT 49.5 Tue 15:15 MA 004

Keldysh nonequilibrium Green's function vs. Feshbach projection operator approach for plasmon-assisted photoemission — •Yaroslav Pavlyukh, Michael Schüler, and Jamal Berakdar — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

A unified theoretical treatment of the single and double electron emission is achieved by using the Feshbach projection method. In this formalism the final target's state fixes the projection operator which subsequently determines the effective Hamiltonian and the optical potential for emitted electrons. The method of non-equilibrium Green's functions is a complementary approach which also allows to treat such processes diagrammatically. We explicitly establish a correspondence between these two approaches and illustrate the diagrammatic technique by calculations of the two-electron emission from C_{60} assisted by the excitation of plasmons.

TT 49.6 Tue 15:30 MA 004

Inclusion of thermal lattice vibrations and spin fluctuations within transport calculations — •Sergiy Mankovsky, Kristina Chadova, Diemo Ködderitzsch, Svitlana Polesya, and Hubert Ebert — Dept. Chemie/Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Deutschland

We present an approach for the calculation of response quantities, e.g. Gilbert damping and electrical conductivity, accounting for temperature induced effects of lattice vibrations and spin fluctuations. The approach is based on the alloy analogy model with thermal vibrations and spin fluctuations modeled by random atomic displacements or magnetic moments deviations, respectively. We discuss various models to deal with spin fluctuations, determining their impact on the temperature dependent behaviour of conductivity and Gilbert damping parameter. We demonstrate the non-additivity of the separate contributions to the conductivity. The results of the calculations are compared to experimental data demonstrating a rather good agreement for the systems under consideration.

TT 50: Graphene (organized by O)

Time: Tuesday 18:15–21:00 Location: Poster A

TT 50.1 Tue 18:15 Poster A

Facile Electrochemical Transfer of Single Crystal Epitaxial Graphene from Ir(111) — Line Koefoed[2], •Antonija Grubišić Čabo[1], Mikkel Kongsfelt[2], Søren Ulstrup[1], Andrew Cassidy[1], Patrick R. Whelan[3], Marco Bianchi[1], Maciej Dendzik[1], Filippo Pizzocchero[3], Bjarke Jørgensen[4], Peter Bøggild[3], Liv Hornekaer[1], Philip Hofmann[1], Steen U. Pedersen[2], and Kim Daasbjerg[2] — [1]Department of Physics and Astronomy and Interdisciplinary Nanoscience Center, University of Aarhus, Ny Munkegade 120, 8000 Aarhus C, Denmark — [2]Department of Chemistry and Interdisciplinary Nanoscience Center, University of Aarhus, Langelandsgade 140, 8000 Aarhus C, Denmark — [3]Department of Micro- and Nanotechnology, Technical University of Denmark, 2800 Kongens Lyngby, Denmark — [4]Newtec A/S, Staermosegårdsvej 18, 5230 Odense M, Denmark

We present an electrochemical method for the transfer of large-area, high-quality single crystalline graphene from Ir(111) to SiO_2/Si under ambient conditions. The method is based on intercalation of tetraoctylammonium ions between the graphene layer and the Ir surface. This simple technique allows transfer of graphene single crystals having the same size as the substrate they are grown on (diameter ≈ 8 mm). In addition, the substrate can be re-used for further growth cycles. A detailed Raman map analysis of the transferred graphene reveals that the initial characteristics and imprints left on the sheet of graphene in terms of strain and wrinkles from the growth process remain after transfer.

TT 50.2 Tue 18:15 Poster A

The influence of the subtrate roughness on the electronic properties of sidewall graphene nanoribbons — •Johannes Aprojanz, Jens Baringhaus, Julia Wiegand, Michael Oestreich, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

Graphene nanoribbons (GNR), epitaxially grown on the sidewalls of silicon carbide (SiC) mesa structures, have shown exceptional transport properties such as ballistic conduction within a single channel and electronic mean free paths of up to 15 μm [1]. We present a detailed study of the growth process of sidewall GNR using scanning probe and electron microscopy as well as Raman spectroscopy. Focussing on the influence of the substrate roughness, the density of terrace steps and the step height can be precisely controlled by a resistive "face-to-face" heating treatment The local electronic properties are investigated by means of a 4-tip STM. The roughness of the SiC and of the mesa sidewalls is identified as detrimental to the electronic performance of sidewall GNR. The mean free path of the ribbons is shown to be directly dependent on the substrate terrace width. For a high density of terrace steps, a transition from ballistic to one dimensional diffusive transport is observed. In addition, Raman spectra show a selective graphene growth on the mesa sidewalls with a I(D)/I(G) ration below 0.1, which indicates high quality graphene nanostructures.

[1] Baringhaus et al., Nature **506**, 349 (2014)

TT 50.3 Tue 18:15 Poster A

Towards the growth of double-layer graphene by conversion of molecular monolayers — •Christof Neumann[1], Gerardo Algara-Siller[2], Daniel Emmrich[1], Marta Trelka[1], Ute Kaiser[2], and Andrey Turchanin[1] — [1]Faculty of Physics, University of Bielefeld, 33615 Bielefeld — [2]Electron Microscopy Group of Materials Science, University of Ulm, 89081 Ulm

Graphene double-layers are desired for implementation of novel electronic and optoelectronic devices as well as for applications in nanofiltration and energy storage. Despite the recent great success in production of single-layer graphene sheets, viable routes to produce graphene double-layers have not been yet established. Here, we present a molecular approach towards graphene double-layers based on the temperature-induced conversion of cross-linked self-assembled monolayers of 1,1',4',1"-terphenyl-4-thiol (TPT) on Cu(111) and polycrystalline copper foils. We characterize this transformation by complementary experimental techniques including X-ray photoelectron and Raman spectroscopy, low energy electron diffraction, helium ion and scanning tunneling microscopy. To determine the structure of suspended graphene nanomembranes we employ high resolution transmission electron microscopy and selected area electron diffraction.

TT 50.4 Tue 18:15 Poster A

Magnetotransport of epitaxial Graphene with single ion-implanted Boron, Nitrogen and Carbon atoms — Philip Willke[1], •Anna Sinterhauf[1], Sangeeta Thakur[3], Julian

A. Amani[2], Thomas Kotzott[1], Steffen Weikert[2], Kalobaran Maiti[3], Hans Hofsäss[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Universität Göttingen, Germany — [2]II. Physikalisches Institut, Universität Göttingen, Germany — [3]Department of Condensed Matter Physics and Materials' Science, TIFR, Mumbai, India

Using magnetotransport (MR) experiments we investigate the transport properties of SiC-Graphene in combination with low-energy ion implantation. Here, we demonstrate the incorporation of single boron, nitrogen and carbon atoms for which the microscopic structure has been additionally studied by scanning tunneling microscopy [1]. The ion-implanted samples exhibit a higher resistance and a lower mobility than undoped samples. Additionally, we find a positive MR for undoped samples switching to a negative MR for doped samples at high magnetic fields, especially for $^{11}B^{+}$- and $^{12}C^{+}$-ions. We explain this behavior with the additional presence of localized scattering centers which we describe in the context of weak localization theory. This work was supported by DFG priority program 1459 "Graphene".

[1] P. Willke et al., Appl. Phys. Lett. 105, 111605 (2014)

TT 50.5 Tue 18:15 Poster A

Local properties of graphene nanoribbons with well-controlled structural variations — •Christian Härtinger, Fabian Queck, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, D-93040 Regensburg

Atomically well-defined graphene nanoribbons can be grown by bottom-up on-surface chemistry [1], which allows for a detailed analysis by scanning probe microscopy and spectroscopy methods. This synthesis can be even extended to grow graphene nanoribbon heterostructures with a local variation of doping [2]. Here, instead we implement local structural variations of a nanoribbon on an Au(111) substrate by introducing suitable precursor molecules in the synthesis process. The influences of these structural variations on the local electronic properties are studied at low temperatures of 5 K by means of scanning probe microscopy and spectroscopy.

[1] Cai et al., Nature 466, 470-473 (2010)
[2] Cai et al., Nature nanotechnology 9, 896-900 (2014)

TT 50.6 Tue 18:15 Poster A

Electronic and transport properties of graphene nanoribbons on Ni(111) — •Bernhard Kretz[1] and Aran Garcia-Lekue[1,2] — [1]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, E-20018 San Sebastian, Spain — [2]IKERBASQUE, Basque Foundation for Science, E-48011 Bilbao, Spain

It is well known that graphene holds a great potential for electronic applications. The graphene-Ni system is an interesting case where the interaction with the ferromagnetic substrate gives rise to a number of remarkable phenomena.[1] In particular, the spin-dependent scattering of electrons at the edges of graphene islands on Ni(111) makes this system very interesting for spintronic devices.[2] Besides, the electron scattering is found to be dependent on the detailed edge structure of the graphene islands, which can exhibit unreconstructed or Stone-Wales reconstructed zigzag edge conformations.[3] In this work, we study the influence of the edge structure on the transport properties across graphene-Ni junctions. We consider graphene nanoribbons on Ni(111) with an unreconstructed and a Stone-Wales reconstructed zigzag edge, both of which are unpassivated, and we use density functional theory (DFT) calculations using the SIESTA and TranSIESTA codes.

[1]V. M. Karpan et al., Phys. Rev. Lett. 99, 176602 (2007); M. Weser et al., APL 96, 012504 (2010)
[2] A. Garcia-Lekue et al., PRL 112, 066802 (2014)
[3] A. Garcia-Lekue et al., submitted

TT 50.7 Tue 18:15 Poster A

Self-assembled PTCDI monolayers for band gap engineering using organic solid/solid wetting deposition — •Oliver Gretz[1,2] and Frank Trixler[1,2,3] — [1]Technische Universität München, School of Education, München, Germany — [2]Zentrum Neue Technologien, Deutsches Museum, München, Germany — [3]Department für Geo- und Umweltwissenschaften & Center for NanoScience, Sektion Kristallographie, Ludwig-Maximilians-Universität München, Germany

Graphene based semiconductors could be fabricated by inducing a band gap at the Dirac point in the graphene band structure. According to theoretical investigations perylene-3,4,9,10-tetra-carboxylic-diimide (PTCDI) is a promising organic semiconductor to open up a band gap in graphene by monomolecular physisorption. However the self-assembly of PTCDI monolayers on graphite could only be shown by epitaxial growth in ultra-high vacuum, yet.

Organic Solid/Solid Wetting Deposition (OSWD) is a process which enables the deposition of insoluble molecules such as organic semiconductors on substrate surfaces under ambient conditions. Here we show first results with PTCDI using OSWD, obtained via scanning tunneling microscopy, which are crucial for tuning the band structure of graphene.

TT 50.8 Tue 18:15 Poster A

Interaction between polycrystalline copper substrate and graphene during atmospheric Chemical Vapor Deposition — •Umut Kamber, Cem Kincal, Hakki Tunç Çiftçi, Berk Zengin, Dilek Yildiz, and Oğuzhan Gürlü — Istanbul Technical University, Istanbul, Turkey

Due to its inevitable potential to be used in wide scale electronics applications, research on high quality, large area, single sheet graphene production became an intense field. For this purpose Chemical Vapor Deposition (CVD) was presented as the most efficient method. In order to obtain defect-free CVD grown graphene sheets, understanding the interaction between graphene and substrate surface is crucial. We observed that graphene can grow over different Cu facets in a continuous film, as reported earlier. Graphene films are depressed near the step-edges of the substrate and moiré patterns occur on some of the atomically flat terraces. Formation of the moiré patterns on only some of the Cu facets indicate differences between the interaction of graphene with different Cu facets. Formation of the graphene on the Cu surface clearly affects the mobility of the Cu atoms on the relevant facet at high temperature. Moreover, we observed that if the copper surfaces are covered by bulk carbon without forming graphene, copper surface crystallizes more properly than graphene covered one. Thus, we claim that formation of graphene effects the crystallization of copper surface, which generates a growth feedback affecting the quality of the graphene film grown.

TT 50.9 Tue 18:15 Poster A

Thickness, roughness and electronic structure characterisation of graphene using soft x-ray reflection spectroscopy — •Christine Jansing[1], Hud Wahab[2], Marc F. Tesch[1,3], Markus Gilbert[1], Andreas Gaupp[1], Andrey Sokolov[3], Dong Hee Shin[4], Suk-Ho Choi[4], Hans-Christoph Mertins[1], Heiko Timmers[2], Dominik Legut[5], and Peter M. Oppeneer[6] — [1]Münster Uni. of Applied Sciences, D-48565 Steinfurt — [2]School of Physical, Environmental and Mathematical Sciences, Uni. of New South Wales Canberra, Canberra, Australia — [3]HZB, D-12489 Berlin — [4]Dep. of Appl. Physics, College of Appl. Science, Kyung Hee Uni., Yongin 446-701, Korea — [5]Nanotechnology Centre, Ostrava, Czech Republic — [6]Depart. of Physics, Uppsala Uni., Uppsala, Sweden

X-ray reflection spectroscopy has been performed on graphene layers supported by different substrates across the C 1s absorption edge. Results confirm that the chemical vapour deposition onto copper foil has produced graphene of monolayer coverage. Graphene, deposited under the same conditions, transferred with a PMMA carrier to other substrate materials, has been measured to be significantly thicker. The interface- and the surface-roughness of the graphene layers have been determined. Structure in the measured reflection spectra can be correlated with ab-initio electronic band structure calculations and assigned to C 1s electron excitations. For the graphene layers transferred to a SiO2 substrate a feature is present that indicates excitation at an energy that is 1.8 eV less than the energy associated with the π^* orbital. This finding is consistent with NEXAFS observations.

TT 50.10 Tue 18:15 Poster A

Preparation of Graphene using the confinement controlled sublimation method — •Cornelis Hilscher, Ulf Berges, Dominique Handschak, Christoph Keutner, Lothar Brosda, Philipp Espeter, and Carsten Westphal — Experimentelle Physik I, TU Dortmund

Graphene is one of the most promising novel materials. Due to rapid, out of equilibrium growth at 1200 °C in ultra high vacuum successfull production of high quality graphene, suitable for electronic applications, still causes many problems. There are some possible solutions like using argon or an enclosure to overcome these issues.

In this work the confinement controlled sublimation method [1] will be used to grow graphene on SiC(0001)-6H. The silicon carbide (SiC)

is surrounded by a graphite enclosure with a small pinhole. Thus, the sublimating silicon stays in the enclosure causing a high silicon vapor pressure during the preparation process. Accordingly, the silicon's sublimation rate is decreased significantly, which leads to a 300 °C increase of the graphene formation temperature. Hence, the growth proceeds near to thermodynamic equilibrium and the graphene layer takes much longer to form. So very homogeneous graphene is expected.

Commissioning and characterization of the preparation chamber is still in progress and includes optimization of parameters like background pressure, heating time and heating temperature.

[1] de Heer, W. A. et al (2011): *Large area and structured epitaxial graphene produced by confinement controlled sublimation of silicon carbide.* In: PNAS, **108**, 41, 16900−16905

TT 50.11 Tue 18:15 Poster A

Polarization doping of graphene on silicon carbide — Samir Mammadov[1], Jürgen Ristein[2], Roland J. Koch[1], Markus Ostler[1], Christain Raidel[1], Martina Wanke[1], Remigijus Vasiliauskas[3], Rositza Yakimova[3], and •Thomas Seyller[1] — [1]Institut für Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany — [2]Lehrstuhl für Laserphysik, FAU Erlangen-Nürnberg, Erwin-Rommel-Str. 1, D-91058 Erlangen, Germany — [3]Department of Physics, Chemistry and Biology, Linköping University, SE-58183, Linköping, Sweden

Being an atomically thin layer, graphene has no bulk. Hence, the charge carier density is influenced by its environment, especially the substrate. While epitaxial graphene on SiC(0001) is n-type doped due to charge transfer from interface states [1], quasi-freestanding graphene (QFG) on H-terminated SiC(0001) is p-type doped [2]. This was explained by the spontaneous polarization of the hexagonal SiC substrate [3]. As a test, we have carried out angle-reolved photoelectron spectroscopy of QFG on H-terminated 3C-SiC(111), 6H-SiC(0001), and 4H-SiC(0001). Using semi-insulating and n-type substrates we shed light on the contributions to the charge carrier density in QFG caused by the spontaneous polarization of the substrate, and the band alignment between the substrate and the graphene layer. In this way we provide quantitative support for the polarization doping model.

[1] S. Kopylov et al., Appl. Phys. Lett. 97 (2010) 112109. [2] F. Speck et al., Appl. Phys. Lett. 99 (2011) 122106. [3] J. Ristein et al., Phys. Rev. Lett. 108 (2012) 246104.

TT 50.12 Tue 18:15 Poster A

Phonon Dispersion of Bilayer Graphene on 6H-SiC(0001) — •Sindy Franz, Christian Heidrich, Roland J. Koch, and Thomas Seyller — Institut für Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany

Electron phonon coupling in graphene leads to characteristic changes in the phonon dispersion as well as a renormalization of the band structure. In the phonon dispersion it results in the well-known Kohn anomalies at the center of the Brillouin zone as well as the K-point. Using high-resolution electron energy loss spectroscopy (HREELS) in off-specular scattering geometry we investigate the phonon dispersion of epitaxial bilayer graphene on silicon carbide. In order to interpret our results, we compare them to previous measurements of monolayer graphene and of the buffer layer.

TT 50.13 Tue 18:15 Poster A

Phonon-Plasmon-Coupling in Bilayer Graphene on 6H-SiC(0001) — •Christian Heidrich, Sindy Franz, Roland Koch, and Thomas Seyller — Institut für Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany

Understanding the interaction between phonons and charge carriers of graphene is of high relevance from a fundamental as well as from an application point of view. Here we report on a study of bilayer epitaxial graphene on SiC(0001) using high resolution electron energy-loss spectroscopy (HREELS). This surface sensitive method is useful for the investigation of phonon vibrations, plasmon excitations, and the coupling of both. It is also possible to study the dispersion of these phenomena over the whole Brillouin zone by varying the scattering geometry. Changing the primary beam energy on the other hand enables measuring those dispersion relations very close to the center of the Brillouin zone. Here we employ the latter to study the coupling of graphene's free charge carrier plasmon to phonons in the substrate as well as graphene itself in the dipole scattering regime. Using dielectric theory calculations, we simulated our measurements and the dispersion relation for the coupled phonon plasmon modes to compare with the experiment.

TT 50.14 Tue 18:15 Poster A

Symmetry broken states of high mobility graphene on boron nitride devices suited for combined transport and STM experiments — •Felix Jekat, Tjorven Johnsen, Nils Freitag, Peter Nemes-Incze, and Markus Morgenstern — II. Physikalisches Institut B, RWTH Aachen, Otto-Blumenthal-Straße, 52074 Aachen

Monolayer graphene is an ideal candidate to combine STM and transport measurements in the Quantum Hall regime. Such measurements require samples in which the exposed graphene surface is clean of processing residues and show high mobility. Here we present magnetotransport measurements of a monolayer graphene on boron nitride prepared by a process which fulfills the above requirements. The sample temperature is as low as 280 mK at a magnetic field of up to 10 T. The presented device shows a field effect mobility of $50,000\,\frac{\mathrm{cm}^2}{\mathrm{Vs}}$. We observe full degeneracy splitting, at a magnetic field of 6 T in the zeroth and first Landau Level within the hole regime and the insulating phase in the zeroth Landau level. In the electron regime, only two fold degeneracy splitting is present. Temperature dependent measurements were conducted to determine the activation gaps of the broken symmetry states revealing gaps up to 80 K.

TT 50.15 Tue 18:15 Poster A

Preparation of high mobility graphene samples for combined transport and STM experiments — •Tjorven Johnsen, Felix Jekat, Nils Freitag, Peter Nemes-Incze, and Markus Morgenstern — II. Physikalisches Institut B, RWTH Aachen, Otto-Blumenthal-Straße, 52074 Aachen

Graphene on boron nitride provides the possibility to measure high mobility two dimensional electron systems by scanning tunneling microscopy. For this kind of measurement clean surfaces are crucial leading to the requirement that the exposed graphene surface has to be clean of processing residues. Adapting a dry transfer method presented by Kretinin et al. [1] for graphene transfer on boron nitride and employing shadow mask evaporation we are able to produce ultra clean graphene surfaces. A graphene flake is placed on a boron nitride flake exfoliated on SiO_2/Si chip serving as the back gate. Charge carrier concentration can thus be controlled during the experiment. The graphene flake ($30\times30\,\mu$m, bubble free area of $10\times10\,\mu$m) is contacted by 50 nm gold contacts defined by shadow mask evaporation. Homemade glass fibers [2] and TEM grids are utilized as shadow masks with alignment precision down to $2\,\mu$m. Four probe transport measurements exhibit high mobility ($50,000\,\frac{\mathrm{cm}^2}{\mathrm{Vs}}$) and symmetry breaking in Quantum Hall Effect at 0.3 K. We also report on the less successful contacting by microsoldering [3].

[1]A. V. Kretinin et al., NanoLett.14, 3270 (2014)
[2]N. Staley et al., Appl. Phys. Lett. 90, 143518 (2007)
[3]V. Geringer et al., Appl. Phys. Lett. 96, 082114 (2010)

TT 50.16 Tue 18:15 Poster A

Polarization-dependent radiation patterns of Raman scattering from Graphene — •Harald Budde, Nicolas Coca Lopez, Xian Shi, and Achim Hartschuh — Department Chemie and CeNS, LMU München, Germany

Raman Scattering Spectroscopy is a powerful technique for studying graphene and other sp2 carbon materials [1]. We combined Raman Spectroscopy with back focal plane (BFP) imaging, a method used to visualize the angular distribution of emitted or scattered light. As an example BFP imaging allows to determine the orientation of single dipolar emitters [2, 3].

Graphene's Raman radiation pattern can be described as the incoherent sum of two orthogonal point dipole emitters despite its extended two-dimensional structure. Parameter-free model calculations using previously reported Raman polarization data are in excellent agreement with the observed radiation patterns of both G and 2D band. We show that the observed polarization ratio of the 2D band and the 2D/G intensity ratio depend on the numerical aperture of the microscope objective used. Finally, the detection efficiency in microscopic Raman measurements is extracted from calculated patterns and is in agreement with the experimental data.

[1] A. Ferrari, D. Basko, Nat. Nanotech. 8, 235-246, 2013.
[2] M. Lieb, J. Zavislan, L. Novotny, J. Opt. Soc. Am. B 21, 1210-1215, 2004.
[3] N. Hartmann, G. Piredda, J. Berthelot, G. Colas des Francs, A. Bouhelier, A. Hartschuh, Nano Lett. 12, 177-181, 2012.

TT 50.17 Tue 18:15 Poster A

Innovative protocols for the epitaxial growth of graphene and boron nitride on Ag(111) — •Manuela Garnica, Felix Bischoff, Yuanqin He, Jacob Ducke, Martin Schwarz, Johannes V. Barth, and Willi Auwärter — Physik Department E20, Technische Universität München, Germany.

In recent years, the research of graphene and other 2D materials has spurred tremendous expectations for potential technological applications. In particular, the chemical vapour deposition (CVD) technique has been shown to be an effective method to grow large-areas of graphene and h-BN on highly reactive metals [1]. However, the low reactivity of nobel metals makes the synthesis of 2D materials using the standard CVD techniques cumbersome [2]. In this work, we explore different growth methods of graphene and h-BN layers on Ag(111) substrates. We combine novel and well-established protocols like CVD, E-Beam evaporation or ion gun assisted deposition. The characterization of the structural properties of these layers was achieved by atomic-scale scanning probe microscopy (STM/AFM). We report the observation of different domain length, edges and defects for the resulting layers. Furthermore, we explore with subnanometer resolution the electronic properties and local surface potential of the layers by means of scanning tunneling spectroscopy.

[1] M. Batzill, Surf. Sci. Rep. 67 (2012), p. 83

[2] B. Kiraly et al. Nat. Commun. 4 (2013) 2804; F. Müller et al. Phys. Rev. B 82, (2010) p. 113406; Martinez-Galera et al, Nano Lett 11, (2011) p3576

TT 50.18 Tue 18:15 Poster A

Transition of image-potential states from free-standing graphene to the graphene/metal interface — •Nico Armbrust, Jens Güdde, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg

We present a theoretical study of the formation of image-potential states on a graphene layer at varying distance to a metal surface. For this purpose we have constructed an analytical one-dimensional model-potential on the basis of the two-band model for the metal and a parametrized potential that reproduces the double Rydberg-like series of even and odd image-potential states of free-standing graphene. This enables us to calculate energies and wavefunctions of the combined system for arbitrary distances between graphene and the metal surface by solving the one-dimensional Schrödinger-equation numerically. For large distances, the image-potential states are typically located at the graphene sheet since its work function is lower than that of most metals. We show, how this double series of free-standing graphene evolves into a single series of the semi-infinite graphene/metal system when a flat graphene layer approaches the metal surface. Our model can quantitatively reproduce experimental data on graphene/Ir(111) and graphene/Ru(0001) which strongly differ in the interaction strength and therefore the binding distance. In particular, the model can explain the different binding energy and lifetime of the first ($n = 1$) image-potential state in the valley and hill areas of the moiré superlattice of graphene/Ru(0001).

TT 50.19 Tue 18:15 Poster A

Structural defects on swift heavy ion irradiated graphitic surfaces — •Cem Kincal[1], Dilek Yildiz[1], Deniz Aşan Acar[1], Clara Grygiel[2], Cornelis J. van der Beek[3], and Oğuzhan Gürlü[1] — [1]Istanbul Technical University, Istanbul, Turkey — [2]Université de Caen, Caen , France — [3]Ecole Polytechnique, Palaiseau, France

Hillock like structures on Highly Oriented Pyrolytic Graphite (HOPG) surfaces due to perpendicular swift heavy ion (SHI) irradiation were previously reported. Our results showed that structures that form on HOPG surfaces due to uranium SHI irradiation in perpendicular geometry have a variety of shapes and sizes rather than just being hillock like. Most of such defects were observed to be distributed on a line rather than being localized to a single point. On the other hand, SHI irradiation of moiré zones on HOPG surfaces under grazing incidence did neither show destruction of the graphene layer generating the moiré pattern, nor any unzipping of the graphene as shown to happen on SHI irradiation of graphene crystals on dielectric substrates. Rather the defects forming as a result of grazing incidence irradiation were comet like both on pristine HOPG samples as well as on moiré domains. Moreover, our irradiation experiments on different graphitic samples showed variations in the structures of the induced defects on the surfaces depending on the crystal quality. Comparison of perpendicular irradiation defects on HOPG terraces to the ones on the moiré domains showed considerable differences.

TT 50.20 Tue 18:15 Poster A

Water chemistry beneath graphene: Formation and breathing of a super-dense OH-H2O phase under graphene — Elin Grånäs[1], •Ulrike A. Schröder[2], Mohammad A. Arman[1], Mie Andersen[3], Timm Gerber[2], Karina Schulte[4], Jesper N. Andersen[1,4], Thomas Michely[2], Bjørk Hammer[3], and Jan Knudsen[1,4] — [1]Division of Synchrotron Radiation Research, Lund University, Sweden — [2]II. Physikalisches Institut, Universität zu Köln, Germany — [3]Interdisciplinary Nanoscience Center and Department of Physics and Astronomy, Aarhus University, Denmark — [4]MAX IV Laboratory, Lund University, Sweden

Placing catalysts in confined environments, e.g. carbon nanotubes, is a powerful method to modify their activity or selectivity. Unfortunately, atomic level understanding of the confinement effects is hindered by the complexity of these materials.

We use Ir(111)-supported graphene (Gr) flakes to study room temperature reduction of atomic oxygen in a confined 2D nano-reactor with X-ray photoelectron spectroscopy and scanning tunneling microscopy. The Gr cover can be used to trap OH-H2O phases that otherwise would desorb directly. Our study of these Gr-stabilized phases and their response to oxygen and hydrogen exposure reveals 2D breathing of a O-OH-H2O phase as O-atoms are dissolved into the structure (expansion) and subsequently converted to OH and H2O (contraction). Using density functional theory calculations combined with a genetic search algorithm, the structure and stability of the trapped OH-H2O structures were determined.

TT 51: Focus Session: Electric Power Applications of Superconductivity

Cuprate high-temperature superconductor (HTS) and MgB_2 based conductor material has meanwhile reached a stage of technical maturity and commercial availability that enables the engineering of many novel high-current applications which are of considerable interest for electric power systems. Topical projects investigate their insertion into established electrical grids in industry and advanced science environments. This Focus Session wants to show which technical achievements have actually been made since the initial euphoria after HTS discovery nearly three decades ago.

Organizers: Bernd Holzapfel (KIT), Roland Hott (KIT), and Kurt Scharnberg (Uni Hamburg)

Time: Wednesday 9:30–12:15 Location: H 0104

Invited Talk TT 51.1 Wed 9:30 H 0104

High Power Equipment based on High-Temperature Superconductors: the Added Value from an Industrial Point of View — •Tabea Arndt, Michael Frank, Jörn Grundmann, Anne Kuhnert, Peter Kummeth, Hans-Peter Krämer, Wolfgang Nick, Marijn Oomen, and Christian Schacherer — Siemens AG, CT RTC PET SUC-DE, Erlangen, Germany

The development and production of High-Temperature Superconductors (HTS) especially in the form of long length wires and tapes has made tremendous progress in the last two decades. A first implication is the steadily increasing number of applications in power technology based on these superconductors. A second implication is that some of the challenges related to the specific devices can not be addressed by academia alone anymore. Nevertheless the industrial players will definitely need support from science and young academics.

This contribution will report on the main properties relevant for application creating 'unique selling points' and the progress in HTS

wires and the technology readiness level of selected devices and applications in power technology (e.g., motors, generators, magnets and fault current limiters).

There are some success stories to be covered. We will comment on remaining challenges in material and in bridging the gap of a 'technology push' to a 'market pull'. Finally an outlook is given on near term applications in power technology.

Topical Talk TT 51.2 Wed 10:00 H 0104

Conductors and Cables from REBCO High Temperature Superconductors for Applications — •Wilfried Goldacker — Karlsruher Institut für Technologie - ITEP, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Deutschland

The availability of commercial REBCO high temperature superconductor (HTS) tapes enables a couple of applications in magnets, current limiters, power lines, transformer and rotating machinery. The HTS material has to be conditioned or assembled to cables for the different applications to achieve the required currents and technical features. The conductor performance, however, is still far from perfection, in particular the homogeneity of the current carrying capacity. Features requested for the specific application are very high operation currents, low AC losses, thermal and mechanical stabilization and filament structures. We review typical REBCO tape features and show the impact on the designs and efforts to develop high current cables from such tapes, including a review of the running investigations in different laboratories. Two of the most promising and advanced cables presented in detail, the Roebel cable and the CORC cable (Conductor on round core), are concepts with transposition of the strands and reduced AC losses. The status of the development, the cable features under different aspects, the achieved transport currents and the future potential are discussed. Finally examples for applications, as HTS fusion or accelerator magnets, are addressed with the related conductor development, followed by conclusions on the expected future potential of the material for such purpose.

Topical Talk TT 51.3 Wed 10:30 H 0104

Power Transmission via Superconducting Lines — •Amalia Ballarino — CERN, 1211 Geneva 23, Switzerland

Superconductivity is an enabling technology for high energy physics. Accelerators made with high field superconducting magnets have allowed ever deeper exploration of the structure of matter over the years culminating in the recent discovery of the Higgs boson at the Large Hadron Collider (LHC) at CERN. This particle accelerator contains 1200 tons of high-performance Nb47Ti superconductor operated at superfluid helium temperature, and it represents today the largest application of superconductivity for high energy physics. An accelerator requires magnets for steering and focusing of the particle beams, but also requires sophisticated equipment for feeding the current from the room temperature environment of the power converters to the cryogenic environment of the associated electrical circuits. To cover this function, novel electrical transfer lines are being developed at CERN in the framework of an upgrade of the LHC to increase the brightness of the interactions. These lines are made using magnesium diboride (MgB_2) and high temperature superconductors, are several hundred meters long, are operated in helium gas at temperatures of up to 25 K, and have a total current-carrying capability of greater than 150 kA. The development done at CERN in the framework of superconducting power transmission for accelerators is presented. The application of this technology to other power transmission systems is also discussed, as well as other electric power applications of superconductivity.

15 min. break.

Invited Talk TT 51.4 Wed 11:15 H 0104

High field transport properties of MBE processed Fe-based superconducting thin films — •Kazumasa Iida — Nagoya University, Japan — IFW Dresden, Germany

It has been reported that Fe-based superconductors show high upper critical fields with low anisotropies at low temperatures [1]. Hence these materials may offer a unique possibility for high field magnet applications. However, only a few reports on high-field transport properties of Co-doped Ba-122 and Fe(Se,Te) have been published and the only one for SmFeAs(O,F) thin films to date [2-4]. In order to use this material class for applications, the knowledge of in-field and its orientation dependence of transport properties in a wide range of external fields need to be clarified. In this talk, I will report on high-field (up to dc 45 T) transport properties of P-doped Ba-122, SmFeAs(O,F) and NdFeAs(O,F) thin films prepared by MBE. Although P-doped Ba-122 has the lowest T_c, self-field J_c of over 6 MA/cm^2 at 4.2 K is recorded, which is the highest value ever reported in Fe-based superconductors. Additionally, in-field performance of P-doped Ba-122 shows comparable to those of NdFeAs(O,F) and SmFeAs(O,F) for $H||c$. On the other hand, both NdFeAs(O,F) and SmFeAs(O,F) exhibited higher J_c for $H||ab$ due to the intrinsic pinning [4]. These results indicate that P-doped Ba-122 is the most promising candidates for high-field magnet applications.

[1] M. Putti et al., Supercond. Sci. Technol. **23**, 034003 (2010)
[2] C. Tarantini et al., Phys. Rev. B **86**, 214504 (2012)
[3] Q. Li, W. Si, and I. K. Dimitrov, Rep. Prog. Phys. **74**, 124510 (2011)
[4] K. Iida et al., Sci. Rep. **3**, 2139 (2013)

Topical Talk TT 51.5 Wed 11:45 H 0104

Advanced Superconducting Power Cable for MV Urban Power Supply — •Frank Schmidt[1], Frank Merschel[2], and Mathias Noe[3] — [1]Nexans Deutschland GmbH, Hannover — [2]RWE Deutschland AG, Essen — [3]Karlsruhe Institute of Technology, Karlsruhe

In recent years the technology of superconducting power cable systems has progressed such that the technical hurdles preparing for commercial applications have been mastered. Several field tests of large scale prototypes for the applications of superconducting cables as well as superconducting fault current limiters have been successfully accomplished and the technology of such systems is ready for commercialization. The presentation will give a detailed overview of the German AmpaCity project. An overview will be given on the development, manufacturing and installion of the 10 kV, 40 MVA HTS system consisting of a fault current limiter and of a 1 km cable in the city of Essen. Since it is the first time that a one kilometer HTS cable system is installed together with an HTS fault current limiter in a real grid application between two substations within a city center area, AmpaCity serves as a lighthouse project. In addition it is worldwide the longest installed HTS cable system so far. It is expected that relatively large technical advances will be made in the future of the comparatively new HTS technology, which in turn will bring associated cost reductions. For this reason, the AmpaCity pilot project in the downtown area of Essen in Germany will be an important step on the way to achieving more widespread application of HTS technology.

TT 52: Superconductivity: Fe-based Superconductors – FeSe and others

Time: Wednesday 9:30–12:30 Location: H 2053

TT 52.1 Wed 9:30 H 2053

Electric transport and magnetic properties of high quality FeSe crystals grown by flux method — •Antonio Leo[1,2], Anita Guarino[1,2], Gaia Grimaldi[2], Massimiliano Polichetti[1,2], Davide Mancusi[1], Armando Galluzzi[1], Krastyo Buchkov[3], Elena Nazarova[3], Angela Nigro[1,2], and Sandro Pace[1,2] — [1]Physics Department, University of Salerno, Salerno, Italy — [2]CNR-SPIN Institute, Salerno Unit, Salerno, Italy — [3]Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria

Among the families of iron-based superconductors, the 11-family is one of the most attractive for high field applications at low temperatures. The optimization of the fabrication processes for thin films and bulks is the first step for producing tapes and cables for practical high power conductors. An essential part of this processes is the characterization of electric transport and magnetic properties. In this work, we present the results of such characterization on high quality FeSe crystals grown following the NaCl/KCl flux technique developed by Mok et al. [B. Mok et al., Crystal Growth & Design vol. 9(7), May 2009, pp. 3260-3264], with few modifications related to the specifications of the fabrication equipment. By magneto-resistance measurements and Vibrating Sample Magnetometry, we investigate the field vs. temperature phase diagrams of the samples, which show critical temperature values which are among the highest values registered for this compound. The pinning activation energy is thus derived as a function of magnetic field in order to evaluate the potential applications of this high quality FeSe compound.

TT 52.2 Wed 9:45 H 2053

Local probe study of superconductivity and ferromagnetism coexisting in Li-intercalated FeSe — •Sirko Kamusella[1], Ursula Pachmayr[2], Fabian Nitsche[2], Felix Brückner[1], Hubertus Luetkens[3], Rajib Sarkar[1], Hans-Henning Klauss[1], and Dirk Johrendt[2] — [1]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department Chemie, Ludwig-Maximilians-Universität München, 81377 München, Germany — [3]Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

The intercalated $[(Li_{1-x}Fe_x)OH](Fe_{1-y}Li_y)Se$ exhibits superconductivity with T_c=43 K and ferromagnetic order of iron moments within the Interlayer at $T_{fm} \approx 10$ K. Similar to P-substituted Eu-122 [1] both ordering phenomena are spatially separated and $T_c > T_{fm}$, but in this compound ferromagnetism arises from 3d-electrons and thus offers huge potential to chemically influence the ferromagnetism and further study coexistence in the iron based superconductors.

Our DFT calculation reveals that the hydroxide layers electron-dope the FeSe layer, but do not disturb its typical Fermi surface topology. Instead, the interlayer's dipolar field continuously penetrates the superconducting volume below 10 K.

Our ^{57}Fe-Mössbauer spectroscopy, ^{7}Li-NMR and μSR data show the interplay of both ordering phenomena and distinguish their origin. Our combined results [2] show, that $[(Li_{1-x}Fe_x)OH](Fe_{1-y}Li_y)Se$ is a rare sample of the formation of a spontaneous vortex phase.

[1] T. Goltz, arXiv:1406.7715.
[2] U. Pachmayr *et al.*, Angewandte Chemie (2014).

TT 52.3 Wed 10:00 H 2053

Magnetoresistance and pressure effects on FeSe single crystals — •Stephan Knöner[1], David Zielke[1], Thomas Wolf[2], Christoph Meingast[2], and Michael Lang[1] — [1]Physikalisches Institut, J.W. Goethe-Universität Frankfurt(M), SPP1458, D-60438 Frankfurt(M), Germany — [2]Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany

Among the various iron-based superconductors, FeSe is of special interest, because of its simple structure without spacing layers. In addition, the system exhibits a structural phase transition at ambient pressure and lacks long-range magnetic order. We present resistivity measurements on the newly synthesized FeSe single crystals under truly hydrostatic He-gas pressure up to 800 MPa and magnetic fields up to 10 T. With this technique we were able to precisely determine the pressure dependence of the superconducting (T_c) and structural transition (T_S) in this pressure region, revealing linear pressure dependences with coefficients of dT_S/dP = -31 K/GPa, higher than previously published results, and dT_c/dP = +5.8 K/GPa, which fits very well to literature data. The resistivity just above the superconducting transition has a linear T-dependence and does not change under pressure. A positive magnetoresistance shows up for magnetic fields applied parallel to the c-axis of the crystal, whereas no effect can be observed with the field parallel to the ab-plane. This magnetoresistance grows significantly in size upon cooling through T_S for all pressures. At low temperatures the size of the magnetoresistance decreases with increasing pressure.

TT 52.4 Wed 10:15 H 2053

Orbital-driven nematicity in FeSe — •Seung-Ho Baek[1], Dmitry Efremov[1], Jong Mok Ok[2], Junsung Kim[2], Jeroen van den Brink[1,3], and Bernd Büchner[1,3] — [1]IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Department of Physics, Pohang University of Science and Technology, Pohang, Korea — [3]Technische Universität Dresden, 01062 Dresden, Germany

An important feature in Fe-based superconductors is that superconductivity occurs in the vicinity of nematic ordering - a lowering of the rotational symmetry preserving time-reversal invariance - as well as of magnetic order. The origin of the nematic symmetry breaking has been heavily debated, because lattice, orbital, and spin degrees of freedom are all directly linked one another from a symmetry point of view, and thus it is challenging to establish which ordering is primary. In this talk, I will present nuclear magnetic resonance (NMR) studies of the high-quality FeSe single crystals, demonstrating that orbital degrees of freedom drives the nematic order.

TT 52.5 Wed 10:30 H 2053

Evidence for a pseudogap and charge density wave in FeSe — •Sahana Roessler[1], Cevriye Koz[1], Ulrich Schwarz[1], Ulrich K. Roessler[2], Frank Steglich[1], Liu Hao Tjeng[1], Peter Thalmeier[1], and Steffen Wirth[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]IFW Dresden, Postfach 270016, 01171 Dresden, Germany

We present scanning tunneling microscopy/spectroscopy (STM/S) and electrical transport measurements on the structurally simple Fe-based superconductor FeSe. This compound displays a structural transition at T_s = 90 K [1,2] and a superconducting transition at T_c = 8.5 K [3]. We show that there is a crossover energy scale at temperature $T^* \approx 70$ K, below which the anisotropic scatterings of the quasiparticles dominate the transport. The magnetization measurements indicate that T^* is also an energy scale of spin fluctuations. A pseudogap associated with a one-dimensional charge density wave (CDW) was observed below 35 K in the STM/S. The CDW is found to coexist with superconductivity. The pseudogap as well as the CDW observed here are reminiscent of behaviors found also in several high-T_c cuprates, strongly suggesting that the spin and charge fluctuations are intimately connected with high-temperature superconductivity.

[1] T. M. McQueen *et al.*,Phys. Rev. Lett. **103**, 057002 (2009).
[2] C. Koz *et al.*, Z. Anorg. Allg. Chem. **640**, 1600-1606 (2014).
[3] F. C. Hsu *et al.*, Proc. Natl. Acad. Sci. U. S. A. **105**, 14262-14264 (2008).

TT 52.6 Wed 10:45 H 2053

Correlation-driven topological Fermi surface transition in FeSe — I. Leonov[1], •S. L. Skornyakov[2,3], V. I. Anisimov[2,3], and D. Vollhardt[1] — [1]TP III, Center for Electronic Correlations and Magnetism, Univ. Augsburg, Germany — [2]Institute of Metal Physics, Yekaterinburg, Russia — [3]Ural Federal Univ., Yekaterinburg, Russia

We present results of a theoretical investigation of the electronic structure and phase stability of paramagnetic FeSe obtained within a combination of *ab initio* methods for calculating band structure and dynamical mean-field theory [1]. Our results reveal an entire reconstruction of the Fermi surface topology upon a moderate expansion of the lattice (Lifshitz transition), with a change of magnetic correlations from the in-plane magnetic wave vector (π, π) to $(\pi, 0)$. We attribute this behavior to a correlation-induced shift of the Van Hove singularity originating from the d_{xy} and d_{xz}/d_{yz} bands at the M-point across the Fermi level. Our results predict a structural transition of FeSe upon a ca. 10% expansion of the lattice volume as well as a topological change of the Fermi surface of FeSe upon partial substitution Se by Te, which is accompanied with a sharp increase of the local moments. We expect

that these changes are responsible for the experimentally observed increase of T_c in FeSe upon doping with Te. The microscopic origin for superconductivity in this system is then due to a Van Hove singularity close to the Fermi level. This identification may open a new route to increase T_c even further.

[1] I. Leonov, S. L. Skornyakov, V. I. Anisimov, D. Vollhardt, arXiv:1411.0604 (2014).

15 min. break.

TT 52.7 Wed 11:15 H 2053

FeSe nano-crystals on Bi_2Se_3(0001) — Sujit Manna[1], Roozbeh Shokri[1], Holger L. Meyerheim[1], Sumalay Roy[1], Katayoon Mohseni[1], •Alberto Cavallin[1], Vasilii Sevriuk[1], Dirk Sander[1], and Jürgen Kirschner[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany.

Iron selenide (FeSe) is a prominent and intensely investigated bulk superconductor owing to its simple tetragonal structure and high transition temperature T_C of 8.5 K [1]. Tremendous activity has aimed to increase T_C by applying pressure, chemical doping, and by a reduction of the structural symmetry [2–4]. Here, we present our LEED, XRD, STM, and STS results on the epitaxial growth of few unit cells thick FeSe nano-crystals on the (0001) surface of the topological insulator Bi_2Se_3. In this case, the substrate induces a uniaxial in-plane strain and lowers the FeSe symmetry from tetragonal to orthorhombic with a b/a ratio of 1.02. STS at 10 K shows a differential conductivity gap at the Fermi energy. Our results open new perspectives for the study of Fe-based superconductivity and of superconductor/topological insulator interfaces in general, by identifying the role of epitaxial strain to modify the atomic structure of FeSe.

[1] F. C. Hsu, et al. Proc. Natl. Acad. Sci. USA 105, 14262 (2008).
[2] Y. Mizuguchi, et al. Applied Phys. Lett. 93, 152505 (2008).
[3] S. Medvedev, et al. Nature Materials 8, 630 (2009).
[4] Q.-Y. Wang, et al. Chin. Phys. Lett. 29, 037402 (2012).

TT 52.8 Wed 11:30 H 2053

Mutual independence of T_c and superfluid density under pressure in optimally-doped $LaFeAsO_{1-x}F_x$ — •Giacomo Prando[1], Ilya Eremin[2], Wolf Schottenhamel[1], Zurab Guguchia[3], Felix Ahn[2], Thomas Hartmann[2], Igor Nekrasov[4], Rustem Khasanov[3], Samuele Sanna[5], Christian Blum[1], Sabine Wurmehl[1,6], and Bernd Büchner[1,6] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany — [2]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [3]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [4]Institute for Electrophysics, RAS, Ekaterinburg, 620016, Russia — [5]Dipartimento di Fisica e Unitá CNISM di Pavia, Universitá di Pavia, I-27100 Pavia, Italia — [6]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany

We report on the effect of nearly-hydrostatic pressure $P \leq 23$ kbar in an optimally-doped $LaFeAsO_{1-x}F_x$ sample. Our results of muon spin rotation show no dependence of T_c on P and, at the same time, a remarkable enhancement of the superfluid density (n_s). This is a dramatic effect, the saturation value of n_s being increased by ~ 30 % at the maximum P value. We provide evidence from density-functional theory (DFT) calculations that this increase should not be associated to an induced change in the fermiology of $LaFeAsO_{1-x}F_x$. Accordingly, we suggest that the experimental data can be explained by assuming a modification of the ratio between intra- and inter-band impurity scattering, only possible in multi-band SC.

TT 52.9 Wed 11:45 H 2053

Superconductivity in the layered iron-germanide YFe_2Ge_2 — Jiasheng Chen[1], Zhuo Feng[2], Yang Zou[1], Peter Logg[1], Giulio Lampronti[3], and •Malte Grosche[1] — [1]Cavendish Laboratory, Cambridge UK — [2]London Centre of Nanotechnology, University College, London UK — [3]Dept. of Earth Sciences, Cambridge UK

In the d-electron system YFe_2Ge_2, an unusually high Sommerfeld ratio of the specific heat capacity $C/T \sim 100$ mJ/(molK^2) and a non Fermi-liquid temperature dependence of the electrical resistivity $\rho \simeq \rho_0 + AT^{3/2}$ signal strong electronic correlations in an anomalous metallic state. Full resistive transitions, DC diamagnetic screening fractions of up to 80% and clear heat capacity anomalies observed at the transition suggest that pure samples of YFe_2Ge_2 superconduct below 1.8 K [1]. Although the nominal Fe valence in YFe_2Ge_2 is the same as in the isostructural iron-arsenides (K/Rb/Cs)Fe_2As_2, which have similar superconducting transition temperatures and a similarly enhanced heat capacity as YFe_2Ge_2, DFT studies suggest that the electronic structure of YFe_2Ge_2 differs substantially from that of the iron-arsenide superconductors, motivating alternative scenarios [2].

[1] Y. Zou *et al*, Physica Status Solidi (RRL) **8,** 928 (2014).
[2] A. Subedi, PRB **89** 024504 (2014);
D. J. Singh, *ibid.* 024505 (2014).

TT 52.10 Wed 12:00 H 2053

Pseudogap from preformed Cooper pairs in a platinum-iron-arsenide superconductor — M. A. Surmach[1], F. Brückner[1], S. Kamusella[1], R. Sarkar[1], P. Y. Portnichenko[1], J. T. Park[2], H. Luetkens[3], P. Biswas[3], W. J. Choi[4], Y. I. Seo[4], Y. S. Kwon[4], H.-H. Klauss[1], and •D. S. Inosov[1] — [1]TU Dresden, Germany — [2]MLZ, Garching, Germany — [3]PSI, Villigen, Switzerland — [4]DGIST, Daegu, Republic of Korea

Using a combination of μSR, INS and NMR, we investigated the novel iron-based superconductor with a triclinic crystal structure $(CaFe_{1-x}Pt_xAs)_{10}Pt_3As_8$ ($T_c = 13$ K). The T-dependence of the superfluid density from our μSR relaxation-rate measurements indicates the presence of two superconducting gaps. According to our INS measurements, commensurate spin fluctuations are centered at the $(\pi, 0)$ wave vector. Their intensity is unchanged across T_c, indicating the absence of a spin resonance typical for many Fe-based superconductors. Instead, we observed a peak in the spin-excitation spectrum around $\hbar\omega_0 = 7$ meV at the same wave vector, which persists above T_c. The temperature dependence of magnetic intensity at 7 meV revealed an anomaly around $T^* = 45$ K related to the disappearance of this new mode. A suppression of the spin-lattice relaxation rate, $1/T_1T$, observed by NMR immediately below T^* without any notable subsequent anomaly at T_c, indicates that T^* could mark the onset of a pseudogap in $(CaFe_{1-x}Pt_xAs)_{10}Pt_3As_8$, which is likely associated with the emergence of preformed Cooper pairs.

TT 52.11 Wed 12:15 H 2053

Superconductivity in 112 type bismuthides and antimonides — Reiner Retzlaff, Alexander Buckow, Jose Kurian, •Soumya Ray, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt, Germany

We report the epitaxial growth of As free and phase pure thin films of the 112-pnictide compounds $LaPd_xPn_2$ (Pn = Sb, Bi) grown onto (100) MgO substrates by molecular beam epitaxy [1,2]. X-ray diffraction, reflection high-energy electron diffraction, and X-ray photoelectron spectroscopy confirm the $HfCuSi_2$ structure of the material with a peculiar pnictogen square net layer. The superconducting transition temperature, T_c, varies little with Pd concentration. $LaPd_xSb_2$ has a higher T_c (3.2 K) by about 20% as compared to $LaPd_xBi_2$ (2.7 K). Fe substitution of Pd leads to a rapid decay of superconductivity. Our results suggest that these superconductors are conventional type II, and that superconductivity occurs in the metal-pnictogen layer as in all iron-pnictide superconductors rather than in the pnictogen square net layer.

[1] A. Buckow, K. Kupka, R. Retzlaff, J. Kurian, and L. Alff, Appl. Phys. Lett. **101**, 162602 (2012).
[2] A. Buckow, R. Retzlaff, J. Kurian, and L. Alff, Supercond. Sci. Technol. **26**, 015014 (2013).

TT 53: Superconductivity: Vortex Physics

Time: Wednesday 9:30–9:45 Location: H 3005

TT 53.1 Wed 9:30 H 3005

High-resolution dichroic imaging of magnetic flux distributions in superconductors with scanning x-ray microscopy — •Stephen Ruoss[1], Claudia Stahl[1], Markus Weigand[1], Gisela Schütz[1], and Joachim Albrecht[2] — [1]Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart — [2]Research Institute for Innovative Surfaces, FINO, Aalen University, Beethovenstraße 1, 73430 Aalen

The penetration of magnetic flux into the high-temperature superconductor YBCO has been observed using a new high-resolution technique based on x-ray magnetic circular dichroism (XMCD). Superconductors coated with thin soft magnetic layers of CoFeB are observed in a scanning x-ray microscope providing cooling of the sample down to 83K under the influence of external magnetic fields. Resulting electrical currents create an inhomogeneous magnetic field distribution above the superconductor which leads to a local reorientation of the ferromagnetic layer [1]. X-ray absorption measurements with circular polarized radiation allows the analysis of the magnetic flux distribution in the superconductor via the ferromagnetic layer [2]. In this work we present first images taken at 83K with high spatial resolution in the nanoscale [3].

[1] C. Stahl et al., EPL 106, 27002 (2014).
[2] C. Stahl et al., Phys. Rev. B 90, 104515 (2014).
[3] S. Ruoß et al., Appl. Phys. Lett., (submitted).

TT 54: Superconductivity: Heterostructures

Time: Wednesday 9:45–11:00 Location: H 3005

TT 54.1 Wed 9:45 H 3005

Quenching long range magnetic excitations in oxygen sublattice reconstructed thin films of $(SrCuO_2)_n/(SrTiO_2)_2$ superlattices — •Marcus Dantz[1], Jonathan Pelliciari[1], Yaobo Huang[1], Debakanta Samal[2], Valentina Bisogni[1], Paul Olalde-Velasco[1], Vladimir Strocov[1], Gertjan Koster[2], and Thorsten Schmitt[1] — [1]Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [2]MESA+ Institute for Nanotechnology, University of Twente

Multi-layered thin cuprate films allow inducing subtle structural changes with which local crystal field and long range magnetic excitations can be finely tuned [1,2]. In $(SrCuO_2)_n/(SrTiO_2)_2$ cuprate superlattices, in particular, a structural transformation from a bulk infinite planar to a sheet-like local domain environment has recently been predicted and subsequently observed [3,4]. Here we present results on the influence of this subtle structural reconstruction on the collective magnetic excitations using high-resolution resonant inelastic x-ray scattering (RIXS) at the Cu L_3 edge. While bulk like infinite layer films exhibit magnon excitations throughout the whole Brillouin zone, decreasing the thickness of the cuprate layers leads to quenching of the magnons starting from the Gamma point successively to the zone boundary, allowing us to study the coherence length of the collective long range magnetic excitations in these cuprate superlattices.

[1] Minola et al. PRB 85 235138 (2012).
[2] Dean et al. Nat. Mater. 11, 850 (2012).
[3] Zhong et al. PRB 85, 121411 (2012).
[4] Samal et al. PRL 111 096102 (2013).

TT 54.2 Wed 10:00 H 3005

On the universality of the "smile"-gap in the Density of States of a chaotic Josephson junction — •Johannes Reutlinger[1], Yuli Nazarov[2], Leonid Glazman[3], and Wolfgang Belzig[1] — [1]University of Konstanz, Department of Physics, 78457 Konstanz, Germany — [2]Kavli Institute of Nanoscience Delft, Delft University of Technology, 2628 CJ Delft, Netherlands — [3]Department of Physics, Yale University, New Haven CT 06511-8499, USA

The superconducting proximity effect strongly modifies the local density of states in chaotic Josephson junctions. Recently we found that besides the well-known minigap a secondary gap appears just below the superconducting gap edge Δ in the limit of a large Thouless energy $E_{\rm Th} \gtrsim \Delta$ [1]. To check the universality of this novel gap phenomenon we study the effect of nonideal contacts and show that the "smile"-gap crucially depends on the transmission eigenvalue distribution [2]. In a next step we use the random matrix method to investigate the "smile"-gap. This allows us to approach the statistics of Andreev levels, going beyond the quasiclassical Greens function method. It turns out that the hard gap edge softens similar to what is already known from the minigap.

[1] J. Reutlinger, L. Glazman, Yu. V. Nazarov, W. Belzig, Phys. Rev. Lett. **112**, 067001 (2014)
[2] J. Reutlinger, L. Glazman, Yu. V. Nazarov, W. Belzig, Phys. Rev. B **90**, 014521 (2014)

TT 54.3 Wed 10:15 H 3005

Thermodynamics of superconducting quantum metamaterials — •Pierre-Luc Dallaire-Demers and Frank Wilhelm-Mauch — Universität des Saarlandes

Left-handed matematerials are capacitively coupled layers of inductive pieces of conductors. These systems are well studied in the context of microwave metamaterials but their full quantum description or their embedding in highly correlated materials like superconductors are still an open problem. Notably, they are known to have a Van Hove singularity in the density of states at low energy and high pseudo-momentum that could effectively couple and condense Cooper pairs. The goal of this research is to analyze the thermodynamical properties of the order parameter of stacked layers of superconductors with a small repulsive Coulomb interaction. A 3D toy model of such a material is mapped to a Fermi-Hubbard lattice. The temperature dependent anomalous correlation functions are computed variationally from a self-energy functional of a small cluster where inter-cluster tunneling is treated perturbatively. The effect of the repulsive interaction on the Cooper pairs binding can then be seen from the momentum distribution of the condensation amplitude. Such a material could potentially be realized with optical lattices or nanoscaled superconductors.

TT 54.4 Wed 10:30 H 3005

Triplet correlations at ferromagnet/superconductor interfaces: Mechanism and implications — •Daniel Fritsch and James F. Annett — H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom

The interface between a ferromagnet and an *s*-wave superconductor offers a rich variety of physical phenomenons due to different intrinsic correlation effects. Even more interesting phenomenons are to be expected if the interface region allows for some kind of spin-flip mechanism, thus generating equal-spin spin-triplet correlations which are compatible with the ferromagnetic exchange field and leading to the observable long-range proximity effect.

Here, we present results based on numerical solutions of the spin-generalised microscopic Bogoliubov−de Gennes equations incorporating a tight-binding model in the clean limit [1-3]. We compare different types of interfaces that have been suggested to generate spin-triplet pairing correlations and discuss implications on the effectiveness.

[1] D. Fritsch and J. F. Annett, New J. Phys. **16**, 055005 (2014).
[2] D. Fritsch and J. F. Annett,
J. Phys.: Condens. Matter **26**, 274212 (2014).
[3] D. Fritsch and J. F. Annett,
Phil. Mag., accepted and published online (2014).

TT 54.5 Wed 10:45 H 3005

Superconducting Spin Valve Effect in Fe/In based heterostructures — •Pavel Leksin[1], Nadir Garifyanov[2], Ilgiz Garifullin[2], Joachim Schumann[1], Vladislav Kataev[1], Oliver Schmidt[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, DE-01171 Dresden, Germany — [2]Zavoisky Physical-Technical Institute, Kazan Scientific Center of Russian Academy of Sciences, 420029 Kazan, Russia

We report on magnetic and superconducting properties of the spin-

valve multilayer system CoOx/Fe1/Cu/Fe2/In. The Superconducting Spin Valve Effect (SSVE) assumes the T_c difference between parallel (P) and antiparallel (AP) orientations of the Fe1 and Fe2 layers' magnetizations. The SSVE value oscillates and changes its sign when the Fe2 layer thickness d_{Fe2} is varied from 0 to 5 nm. The SSVE value is positive, as expected, in the range 0.4 nm $\leq d_{Fe2} \leq$ 0.8 nm. For a rather broad range of thicknesses 1 nm $\leq d_{Fe2} \leq$ 2.6 nm the SSVE has negative sign assuming the inverse SSVE. Moreover, the magnitude of the inverse effect is larger than that of the positive direct effect. We attribute these oscillations to a quantum interference of the cooper pair wave functions in the magnetic part of the system. For most of the spin-valve samples from this set we experimentally realized the full switching between normal and superconducting states due to direct and inverse SSVE. The analysis of the experimental data has enabled the determination of all microscopic parameters of the studied system [1].

[1] P. V. Leksin et al., Phys. Rev. B 85, 024502 (2012).

TT 55: Low-Dimensional Systems: 2D – Theory

Time: Wednesday 9:30–13:00 Location: H 3010

TT 55.1 Wed 9:30 H 3010

Heat diffusion in the disordered Fermi and electron liquids: The role of inelastic processes — •Georg Schwiete[1] and Alexander Finkel'stein[2,3] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz — [2]Texas A&M University, College Station, US — [3]The Weizmann Institute of Science, Rehovot, Israel

We study thermal transport in the disordered Fermi and electron liquids at low temperatures. Gravitational potentials are used as sources for finding the heat density and its correlation function. For a comprehensive study, we extend the renormalization group (RG) analysis developed for electric transport by including the gravitational potentials into the RG scheme. Our analysis reveals that for the disordered Fermi liquid the Wiedemann-Franz law remains valid even in the presence of quantum corrections caused by the interplay of diffusion modes and the electron-electron interaction. In the present scheme this fundamental relation is closely connected with a fixed point in the multiparametric RG flow of the gravitational potentials. For the disordered electron liquid we additionally analyze inelastic processes induced by the Coulomb interaction at sub-temperature energies. While the general form of the correlation function has to be compatible with the energy conservation, these inelastic processes are at the origin of logarithmic corrections violating the Wiedemann-Franz law. The evolution of various terms in the heat density-heat density correlation function therefore differs from that for densities of other conserved quantities, such as total number of particles or spin.

TT 55.2 Wed 9:45 H 3010

First-principles analysis of MoS_2/Ti_2C and MoS_2/Ti_2CY_2 (Y = F and OH) all-2D semiconductor/metal contacts — •Udo Schwingenschlögl[1], Li-Yong Gan[1], Yu-Jun Zhao[2], and Dan Huang[3] — [1]KAUST, Thuwal 23955-6900, Saudi Arabia — [2]South China University of Technology, Guangzhou 510640, People's Republic of China — [3]Hunan University of Arts and Science, Changde 415000, People's Republic of China

First-principles calculations are used to explore the geometry, bonding, and electronic properties of MoS_2/Ti_2C and MoS_2/Ti_2CY_2 (Y = F and OH) semiconductor/metal contacts. The structure of the interfaces is determined. Strong chemical bonds formed at the MoS_2/Ti_2C interface result in additional states next to the Fermi level, which extend over the three atomic layers of MoS_2 and induce a metallic character. The interaction in MoS_2/Ti_2CY_2, on the other hand, is weak and not sensitive to the specific geometry, and the semiconducting nature thus is preserved. The energy level alignment implies weak and strong n-type doping of MoS_2 in MoS_2/Ti_2CF_2 and $MoS_2/Ti_2C(OH)_2$, respectively. The corresponding n-type Schottky barrier heights are 0.85 and 0.26 eV. We show that the MoS_2/Ti_2CF_2 interface is close to the Schottky limit. At the $MoS_2/Ti_2C(OH)_2$ interface, we find that a strong dipole due to charge rearrangement induces the Schottky barrier. The present interfaces are well suited for application in all-two-dimensional devices.

[1] Phys. Rev. B 87, 245307 (2013).

TT 55.3 Wed 10:00 H 3010

Phase diagram of an extended quantum dimer model on the hexagonal lattice — Thiago Milanetto Schlittler[1], •Thomas Barthel[2], Grégoire Misguich[3], Julien Vidal[1], and Rémy Mosseri[1] — [1]LPTMC, Université Paris-6 — [2]LPTMS, Université Paris-Sud — [3]IPhT, CEA Saclay

We introduce a generalized quantum dimer model on the hexagonal lattice. In addition to the standard Rokhsar-Kivelson Hamiltonian, it contains a competing potential term. The phase diagram is studied by means of quantum Monte-Carlo simulations, variational ansätze and perturbation theory. The model displays a rich phase diagram and, in particular, provides a microscopic realization for the Cantor deconfinement scenario – a cascade of phases with varying flux.

TT 55.4 Wed 10:15 H 3010

The spectra of integrable staggered $sl(2|1)$ network models — •Andreas Klümper[1] and Michael Brockmann[2] — [1]Universität Wuppertal, Theoretische Physik, Gauss-Strasse 20, 42119 Wuppertal — [2]Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1090 GL Amsterdam

We investigate the spectra of transfer matrices of integrable Chalker-Coddington like network models with $sl(2|1)$ symmetry and staggered $3-\bar{3}$ representations. Related to these network models are integrable superspin chains. The research on these models is motivated in general by the spin quantum Hall effect.

There are two kinds of integrable staggered $sl(2|1)$ models : (i) a rather well understood system based on the Temperley-Lieb algebra, (ii) a system based on the Hecke algebra and introduced by R. M. Gade in 1998. The latter model satisfies nested Bethe ansatz equations and was investigated extensively and particularly numerically by Essler, Frahm, Saleur in 2005.

We aim at an analytical treatment of the nested Bethe ansatz equations and derive a closed finite set of non-linear integral equations. These equations are well-posed and valid for any system size as well as for the largest and next-largest eigenvalues of the transfer matrix. The numerical treatment is delicate as straight forward iterations do not converge. However, the equations allow for analytical calculations of conformal properties.

TT 55.5 Wed 10:30 H 3010

Non-Fermi-liquid behavior in a 2D transport model with boson affected hopping — •Dai-Ning Cho and Steffen Sykora — Institute for Theoretical Solid State Physics, IFW Dresden, D-01069 Dresden, Germany

Charge transport mediated by excitations in a correlated background medium is a general phenomenon in condensed matter physics. A simplified model of spinless fermions which are dynamically coupled to a system of bosonic degrees of freedom has been introduced by Edwards. In our work we study the half-filled Edwards model in 2D by use of the projective renormalization method (PRM), which transforms the model Hamiltonian to a solvable effective Hamiltonian involving renormalized bosons and fermions. We find significant reduction of the one-particle spectral weight close to the charge density wave (CDW) phase, which is well-known from the 1D case. Inside this non-Fermi-liquid region an unconventional superconducting phase with s± pairing symmetry is also found. Thereby, the pairing is stabilized by strong renormalization of the charge carrier transport. We present results for the renormalized dispersions and one-particle spectral functions.

TT 55.6 Wed 10:45 H 3010

Two–parameter scaling theory of transport near a spectral node — •Andreas Sinner — Universität Augsburg

We investigate the finite–size scaling behavior of the conductivity in a two–dimensional Dirac electron gas within a chiral sigma model. Based on the fact that the conductivity is a function of system size times scattering rate, we obtain a two–parameter scaling flow toward a finite fixed point. The latter is the minimal conductivity of the infinite system. Depending on boundary conditions, we also observe unstable fixed points with conductivities much larger than the experimentally

observed values, which may account for results found in some numerical simulations. By including a spectral gap we extend our scaling approach to describe a metal–insulator transition.

TT 55.7 Wed 11:00 H 3010

Composite boson mean-field theory for strongly correlated systems — •Daniel Huerga[1,2] and Jorge Dukelsky[1] — [1]Instituto de Estructura de la Materia, C.S.I.C., Madrid, Spain — [2]Institut fur Theoretische Physik III, University of Stuttgart, Stuttgart, Germany

We present a method applicable to spin and bosonic model Hamiltonians of strongly correlated systems. The method is based on the identification of clusters of the original spin and bosonic degrees of freedom as the building blocks which capture the essential quantum correlations to describe the phases emerging in the model. We present a canonical mapping which relates the original spin and bosonic operators to a new set of composite boson (CB) operators that describe the quantum states of the cluster. As the mapping is canonical, we can rewrite the original Hamiltonian in terms of CBs and approach it by standard many-body techniques, with the advantage that short-range correlations are computed exactly from the onset.

A simple Gutzwiller wave function of CBs allows us to uncover the phase diagram of two-dimensional frustrated models such as a model of spins with ring-exchange interaction, or a system of bosons in the presence of artificial magnetic fields. A Bogoliubov approach to the CB quantum fluctuations allows us to accurately describe the recently measured Higgs and Goldstone excitation modes of a system of cold atoms loaded in a two-dimensional optical lattice. The algebraic framework set by the mapping allows for further extensions of the method.

15 min. break.

TT 55.8 Wed 11:30 H 3010

Dimensional-Crossover-Driven Mott Transition: A Variational Plaquette Study — •Benjamin Lenz[1], Salvatore R. Manmana[1], Marcin Raczkowski[2], Thomas Pruschke[1], and Fakher F. Assaad[3] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37073 Göttingen, Germany — [2]Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, D-80333 München, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Recently the metal-insulator Mott transition has been studied for a quasi-two-dimensional frustrated Hubbard model with next-nearest-neighbor hopping [Raczkowski, Assaad, PRL 109 (2012)]. Following up on this CDMFT study at finite temperatures, we analyze the crossover-driven Mott transition at zero temperature by means of variational cluster approximation (VCA). Here, we focus on coupling bath sites to the correlated sites of the reference system to carefully investigate the order of the transition. The effects of this extension on the phase diagram are studied and the insulator-metal transition is found to be of first order for large and intermediate inter-chain coupling strengths. This allows us to pursue the transition to small coupling strengths where remnant 1D effects like Umklapp scattering are expected to become important.

TT 55.9 Wed 11:45 H 3010

Ground state phase diagram of the bilayer square lattice at half filling — •Michael Golor[1], Timo Reckling[1,2], Laura Classen[2], Michael M. Scherer[2], and Stefan Wessel[1] — [1]Institut für Theoretische Festkörperphysik, RWTH Aachen — [2]Institut für Theoretische Physik, Universität Heidelberg

We employ a combination of functional renormalization group calculations and projective determinantal quantum Monte Carlo simulations to examine the Hubbard model on the square lattice bilayer at half filling. We obtain a comprehensive account on the ground state phase diagram with respect to the extent of the system's metallic and (antiferromagnetically ordered) Mott-insulating as well as band-insulating regions. We discuss the difficulty in exploring the weak-coupling regime with quantum Monte Carlo and identify the non-interacting system's Fermi surface as its origin.

TT 55.10 Wed 12:00 H 3010

FRG study of the Hubbard model on the bilayer square lattice — •Timo Reckling[1,2], Michael M. Scherer[2], and Laura Classen[2] — [1]Institut für Theoretische Festkörperphysik, RWTH Aachen University, 52056 Aachen, Germany — [2]Institut für Theoretische Physik, Universität Heidelberg, 69120 Heidelberg, Germany

We study Hubbard model on the bilayer square lattice at and away from half filling as a model unifying various aspects of the physics of two-dimensional correlated fermions. We discuss on-site and interlayer density-density interactions by means of an unbiased functional renormalization group approach. This allows us to deduce the emergent order without previous assumptions about its nature and symmetry and can therefore be used to establish the appearance of spin and charge density wave ordering, as well as two types of superconductive instabilities away from half filling.

TT 55.11 Wed 12:15 H 3010

Mott physics in the half-filled Hubbard model on a family of vortex-full square lattices — •Dominik Ixert[1], Fakher Assaad[2], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik 1, TU Dortmund, D-44221 Dortmund, Germany — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We study the half-filled Hubbard model on a one-parameter family of vortex-full square lattices ranging from the isotropic case to weakly coupled Hubbard dimers. The ground-state phase diagram consists of four phases: A semimetal and a band insulator which are connected to the weak-coupling limit, and a magnetically ordered Néel phase and a valence bond solid (VBS) which are linked to the strong-coupling Mott limit. The phase diagram is obtained by quantum Monte Carlo (QMC) and continuous unitary transformations (CUTs). The CUT is performed in a two-step process: Nonperturbative graph-based CUTs are used in the Mott insulating phase to integrate out charge fluctuations. The resulting effective spin model is tackled by perturbative CUTs about the isolated dimer limit yielding the breakdown of the VBS by triplon condensation. We find three scenarios when varying the interaction for a fixed anisotropy of hopping amplitudes: (i) one direct phase transition from Néel to semimetal, (ii) two phase transitions VBS to Néel and Néel to semimetal, or (iii) a smooth crossover from VBS to the band insulator. Our results are consistent with the absence of spin-liquid phases in the whole phase diagram.

[1] D. Ixert, F. F. Assaad, and K. P. Schmidt,
PRB **90**, 195133 (2014).

TT 55.12 Wed 12:30 H 3010

Entanglement properties of one- and two-dimensional quantum Ising and XXZ spin-1/2 models — •Briissuurs Braiorr-Orrs[1], Michael Weyrauch[1], and Mykhailo Rakov[2] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany — [2]Kyiv National Taras Shevchenko University, 64/13 Volodymyrska st., 01601 Kyiv, Ukraine

Entanglement properties of 1D (spin rings) and 2D (on a square lattice) spin-1/2 quantum Ising and XXZ models are investigated. Numerical methods (MPS in 1D and TERG and CTMRG in 2D) with imaginary-time evolution are used to model the ground state of the studied models. Different entanglement measures, such as one-site entanglement entropy, one-tangle, concurrence of formation and assistance, negativity and entanglement per bond are calculated and their 'characterizing power' to determine the phase transition is compared. A special emphasis is made on the connection of the symmetry properties of the ground states and the entanglement properties of the states.

TT 55.13 Wed 12:45 H 3010

Lattice Conformal Blocks and Topological Phases — •Roberto Bondesan — THP, Cologne, Germany

Conformal blocks are holomorphic building blocks of correlation functions of 2D conformal field theories. The Moore-Read approach relates these objects to the ground state wave functions in the fractional quantum Hall effect. In this talk I will present a lattice perspective on this approach. In particular I will discuss how to use vertex models of statistical mechanics to achieve a tensor network states description of strongly interacting chiral topological phases.

TT 56: Correlated Electrons: Quantum-Critical Phenomena – Theory

Time: Wednesday 9:30–13:15 Location: A 053

TT 56.1 Wed 9:30 A 053

Superconductivity and charge order near the onset of antiferromagnetism in metals — •Max Henner Gerlach[1], Yonathan Schattner[2], Simon Trebst[1], and Erez Berg[2] — [1]University of Cologne, Germany — [2]Weizmann Insitute of Science, Rehovot, Israel

The quantum-critical transition of a system of itinerant electrons into an antiferromagnetically ordered phase has long been believed to play an important role in the physics of superconductors such as the electron-doped cuprates and the iron pnictides. The complete understanding of this quantum-critical point has remained a key challenge for both analytical and numerical approaches. On the computational side, a numerically exact simulation of such fermionic systems via quantum Monte Carlo studies has long been precluded by the infamous negative sign problem. Only recently a way has been found to set up sign-problem-free simulations of lattice models that realize the universal physics close to this phase transition [1].

Building upon this conceptual work, we introduce further improvements to the Monte Carlo sampling techniques adapted to such a model, allowing us to better understand the properties of the quantum-critical point and the instability towards d-wave-like superconductivity in its vicinity. In addition, we study a competing instability towards a charge-density-wave-like order, which we support by a supplementary interaction. Taken together, our results further improve our understanding of the rich physics of a relatively simple single-band electron model appropriate for the cuprates.

[1] E. Berg, M. A. Metlitski, and S. Sachdev, Science **338**, 1606 (2012)

TT 56.2 Wed 9:45 A 053

Quantum Critical Transitions in Spin and Charge Ordered Systems — •Corentin Morice[1], Premala Chandra[2], Stephen E. Rowley[1], and Siddharth S. Saxena[1] — [1]University of Cambridge, Cambridge, United Kingdom — [2]Rutgers University, Piscataway, New Jersey, USA

This talk will focus on search and discovery of novel forms of quantum order in ferroelectric and multiferroic systems. Materials tuned to the neighbourhood of a zero temperature phase transition often show the emergence of novel quantum phenomena. Much of the effort to study these new emergent effects, like the breakdown of the conventional Fermi-liquid theory in metals has been focused in narrow band electronic systems. But Spin or Charge ordered phases in insulating systems can also be tuned to absolute zero. Close to such a zero temperature phase transition, physical quantities like susceptibility change into unconventional forms due to the fluctuations experienced in this region giving rise to new kinds ordered states.

TT 56.3 Wed 10:00 A 053

Interference of quantum critical excitations and soft diffusive modes in a disordered antiferromagnetic metal — •Philipp Weiss[1], Boris Narozhny[1], and Jörg Schmalian[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Germany

We study a two-dimensional metallic system close to an antiferromagnetic critical point within the framework of the spin-fermion model. The model describes fermionic quasiparticles interacting with bosonic collective spin modes close to the antiferromagnetic wave vector $\vec{Q}$. Since $\vec{Q}$ is a large momentum scale, in first order of the spin-fermion coupling, low-energy fermions are only coupled to spin fluctuations at "hot spots" of the Fermi surface which are connected by $\vec{Q}$. However, at second order a fermion at an arbitrary point of a generic Fermi surface can be scattered successively by two spin fluctuations via an intermediate high-energy state and, in total, suffer only a small momentum transfer. This gives rise to an interference of critical spin fluctuations and diffusive excitations of the disordered metal. Integrating out the fermionic high-energy modes above a certain low-energy cutoff, we derive an effective low-energy action which exhibits a local interaction vertex for low-energy fermions on the entire Fermi surface. This interaction is mediated by a composite propagator. Using a diagrammatic approach, we calculate the temperature-dependent interaction correction to dc-conductivity induced by the composite propagator in the presence of disorder and find a correction to residual resistivity.

TT 56.4 Wed 10:15 A 053

Disorder-driven Coulomb gas transitions in classical three-dimensional dimer models — •Stefan Wolff[1,2] and Simon Trebst[2] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Bonn, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Germany

Frustrated magnets can harbor emergent Coulomb phases at low temperatures that exhibit a characteristic power-law decay of correlations and an extensive ground-state manifold. Here we discuss this physics in the context of classical dimer models – prototypical systems that allow to directly study such Coulomb phases. Our focus is on the effect of disorder, which we model by successive percolation of the bonds in a family of three-dimensional lattices with varying coordination number. Notably, our large-scale numerical simulations clearly demonstrate that the break-down of the Coulomb phase is well separated from the percolation transition. We discuss the order of the various phase transitions and the nature of the intermediate phase.

TT 56.5 Wed 10:30 A 053

Dimensionless ratios at the honeycomb Hubbard model critical point — •Thomas C. Lang[1] and Ribhu K. Kaul[2] — [1]Boston University, Boston, USA — [2]University of Kentucky, Lexington, USA

We study the nature and location of the phase transition between the semi-metal and Mott insulating antiferromagnetic state in the half-filled Hubbard model on the honeycomb. Using unbiased quantum Monte Carlo simulations, we measure dimensionless fermionic correlation and magnetic ratios, which provide precise and independent estimates for the couplings at which a mass gap opens in the single particle spectrum and at which the magnetic order sets in. An analysis of our data provides evidence for a direct continuous critical point between the semi-metal and the antiferromagnet, and an accurate window for the critical coupling, which does not include any of the previous estimates for the onset of magnetic order.

TT 56.6 Wed 10:45 A 053

Deconfined quantum criticality beyond designer Hamiltonians — •Ribhu K. Kaul[1] and Thomas C. Lang[2] — [1]University of Kentucky, Lexington, USA — [2]Boston University, Boston, USA

The SU(6) symmetric generalization of the Hubbard model on the square lattice constitutes a candidate for a direct, continuous quantum phase transition from Néel to valence bond solid (VBS) order. By constructing dimensionless quantities such as ratios of the magnetic structure factor and valence bond correlations we are able to unambiguously determine the existence of weak, but robust antiferromagnetic order in the weak coupling regime and a plaquette VBS in the strong coupling limit. Furthermore these ratios provide a tool to accurately determine the (critical) point from both sides of the phase transition separating the two limits. Preliminary results suggest a direct continuous transition for which we extract basic estimates for the critical exponents and compare the scaling function with results from designer SU(6) spin models to investigate whether this quantum phase transition is compatible with the scenario of deconfined quantum criticality.

TT 56.7 Wed 11:00 A 053

Universal phase diagram of quantum dissipative many-body systems — •Gianluca Rastelli — Fachbereich Physik & Zukunftskolleg, Universität Konstanz, D-78457 Konstanz, Germany

The interplay between quantum dissipation and interactions in quantum many-body systems can give rise to a wealth of novel phenomena. The one-dimensional coplanar rotor model (also known as quantum phase model) is a paradigmatic model for studying quantum phase transitions with dissipative coupling to an external bath. It can describe, for instance, one-dimensional chains of superconducting islands connected by Josephson junctions and shunt resistances [1]. At zero temperature, a quantum phase transition occurs by tuning the interaction strength between the phases. When the system is coupled to the environment, the common accepted scenario is that the dissipation suppresses the quantum fluctuations and, therefore, enhances the classical ground state characterised by long-range order [2,3]. Contrary to previous studies, I focus on a system which is coupled to the environment with a dissipative interaction designed in way to reduce the

quantum fluctuations of the conjugate variables of the local phases. I will show that this anomalous dissipation leads to a reversed behaviour of the phase diagram: Increasing the dissipation causes a stabilisation of the disordered quantum ground state.

[1] R. Fazio and H. van der Zant, Phys. Rep. 355, 235 (2001).
[2] S. Chakravarty, G.L. Ingold, S. Kivelson, and A. Luther, Phys. Rev. Lett. 56, 2303 (1986).
[3] P. A. Bobbert, R. Fazio, G. Schön, and G. T. Zimanyi, Phys. Rev. B 41, 4009 (1990).

15 min. break.

TT 56.8 Wed 11:30 A 053

Phase diagram of the Kane-Mele-Coulomb model — •Martin Hohenadler[1], Francesco Parisen Toldin[1], Fakher F. Assaad[1], and Igor F. Herbut[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Department of Physics, Simon Fraser University, Burnaby, Canada

We determine the phase diagram of the Kane-Mele model with a long-range Coulomb interaction using an exact quantum Monte Carlo method. Long-range interactions are expected to play a role in honeycomb materials because the vanishing density of states in the semimetallic weak-coupling phase suppresses screening. According to our results, the Kane-Mele-Coulomb model supports the same phases as the Kane-Mele-Hubbard model. The nonlocal part of the interaction promotes short-range sublattice charge fluctuations, which compete with antiferromagnetic order driven by the onsite repulsion. Consequently, the critical interaction for the magnetic transition is significantly larger than for the purely local Hubbard repulsion. Our numerical data are consistent with $SU(2)$ Gross-Neveu universality for the semimetal to antiferromagnet transition, and with 3D XY universality for the quantum spin Hall to antiferromagnet transition.

[1] M. Hohenadler, F. Parisen Toldin, I. F. Herbut, and F. F. Assaad, Phys. Rev. B 90, 085146 (2014)

TT 56.9 Wed 11:45 A 053

Fermionic quantum criticality in honeycomb and π-flux Hubbard models — •Francesco Parisen Toldin[1], Martin Hohenadler[1], Fakher F. Assaad[1], and Igor F. Herbut[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Department of Physics, Simon Fraser University, Burnaby, Canada

We numerically investigate the critical behavior of the Hubbard model on the honeycomb and the π-flux lattice, which exhibits a direct transition from a Dirac semimetal to an antiferromagnetically ordered Mott insulator. We use projective auxiliary-field quantum Monte Carlo simulations and a careful finite-size scaling analysis that exploits improved renormalization-group invariant observables. This approach, which is successfully verified for the 3D XY transition of the Kane-Mele-Hubbard model, allows us to extract estimates for the critical couplings and the critical exponents. The results confirm that the critical behavior for the semimetal to Mott insulator transition in the Hubbard model belongs to the Gross-Neveu-Heisenberg universality class on both lattices.

[1] F. P. Toldin, M. Hohenadler, F. F. Assaad, I. F. Herbut, arXiv:1411.2502

TT 56.10 Wed 12:00 A 053

Spin Dynamics of the Heisenberg Bilayer from Quantum Monte Carlo — •Maximilian Lohöfer[1], Stefan Wessel[1], Frederic Mila[2], Tommaso Coletta[2], and Fakher Assaad[3] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen — [2]Institut de théorie des phénomènes physiques, Ecole polytechnique fédérale de Lausanne — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg

The spin-1/2 Heisenberg model on the square lattice blayer provides a basic example to study quantum critical behavior in interacting quantum spin systems. While its static equilibrium properties have been intensively investigated in the past, thus far only few studies have discussed the details of the reconstruction of the excitation spectrum across the quantum phase transition between the antiferromagnetically ordered phase and the quantum disordered regime. Here, based on stochastic series expansion quantum Monte Carlo (SSE) simulations and stochastic analytic continuation (SAC) methods, we calculate the dynamical spin structure factors in this model in different symmetry sectors. We analyse the evolution of the low-energy modes, related to Goldstone modes as well as the longitudinal amplitude mode in the ordered phase upon crossing through the quantum critical point and consider the corresponding restoration of the SU(2) symmetry in the disordered regime. The obtained spectra are also discussed in view of results from series expansions, improved spin wave theory and strong-dimer perturbation theory.

TT 56.11 Wed 12:15 A 053

Anomalous dynamical exponent at the Ising-nematic quantum critical point — •Tobias Holder and Walter Metzner — Max-Planck-Institute for Solid State Research, D-70569 Stuttgart, Germany

We present a systematic study of higher order fluctuation corrections for a two-dimensional critical metal at the onset of Ising-nematic order. This type of instability is of interest in the study of competing orders in high-temperature superconductivity and with spin liquids. In the critical regime, strong forward scattering gives rise to non-Fermi liquid behavior with overdamped quasiparticles and a dynamical critical exponent $z = 3$.

Using a renormalization group approach to the spin-fermion model in a two-patch approximation, we analyze the structure of density-density vertices of any order. This allows for a general classification of finite and singular contributions, which reveals a renormalization of $z = 3$ at four loop order. The results are applicable to a wide range of non-Fermi liquids.

TT 56.12 Wed 12:30 A 053

Selfconsistent Renormalization Group for Kondo Breakdown in Kondo lattice or Multi-Impurity Systems — •Ammar Nejati, Katinka Ballmann, and Johann Kroha — Universität Bonn

The conditions for breakdown of Kondo quasiparticles near a heavy-fermion quantum phase transition are still a controversial issue. We present a renormalization group (RG) theory for the breakdown of Kondo screening in multi-impurity Kondo systems without direct interimpurity dipole coupling, without pre-assumptions about magnetic ordering or Fermi surface criticality. Kondo singlet formation is signalled by the RG divergence of the conduction electron – local Kondo spin vertex Γ at the Kondo scale T_K. In a multi-impurity system, Γ acquires a non-local, RKKY-mediated contribution from conduction electrons scattering at surrounding Kondo sites, which depends on the dynamical, local spin response χ on those sites. Because of its inverse dependence on T_K at low energies, $\chi = (g\mu_B)^2/T_K$, the $\beta-$function depends parametrically on the Kondo scale in a selfconsistent way. As a result, we find a universal suppression of the Kondo scale $T_K(y)$ in Kondo lattice and multi-impurity systems, depending on a dimensionless RKKY coupling parameter y. Local Kondo screening is predicted to break down at a maximum RKKY coupling y_{max}, where y_{max} is a universal function of the bare $T_K(0)$. At the breakdown point, the T_K-suppression assumes the universal value $T_K(y_{max})/T_K(0) = 1/e \approx 0.368$, in remarkable quantitative agreement with STM spectroscopy on two-impurity systems [1].

[1] J. Bork *et al.*, Nature Physics **7**, 901 (2011).

TT 56.13 Wed 12:45 A 053

Steady state dynamics and effective temperatures of quantum criticality in open systems — •Farzaneh Zamani[1], Pedro Ribeiro[2], and Stefan Kirchner[3] — [1]Max Planck Institute for Physics of Complex Systems, 01187 Dresden, Germany — [2]Russian Quantum Center, Business-center "Ural", Novaya street 100A, Skolkovo village, Odintsovo district, Moscow area, 143025 Russia — [3]Center for Correlated Matter, Zhejiang University, China

We present our results for the steady-state –both thermal and non-thermal– scaling functions and steady-state dynamics in a quantum impurity model of local quantum criticality. Our model, the pseudo-gap Kondo model, allows us to obtain full scaling functions in and out of equilibrium. We discuss the (equilibrium) zero-temperature residual entropy at various fixed points. We also consider the non-equilibrium steady-state, obtained by applying a finite bias voltage and study the concept of effective temperatures near fully interacting as well as weak-coupling fixed points. In the vicinity of each fixed point we establish the existence of an effective temperature –different at each fixed point– such that the equilibrium fluctuation-dissipation theorem is recovered. Interestingly, steady-state scaling functions in terms of the effective temperatures coincide with the equilibrium scaling functions in terms of the temperature. This result extends to higher correlation functions as is explicitly demonstrated for the Kondo singlet strength. We also

study the non-linear charge transport in terms of the effective temperatures.

TT 56.14 Wed 13:00 A 053

Spin-orbit coupling in interacting quantum wires — •Nikolaos Kainaris[1,2] and Sam T. Carr[3] — [1]Institut für Theorie der Kondensierten Materie, KIT Karlsruhe, Germany — [2]Institut für Nanotechnologie, KIT Karlsruhe, Germany — [3]School of Physical Sciences, University of Kent, Canterbury, United Kingdom

We present analysis of the interacting quantum wire problem in the presence of spin-orbital interaction. We find that the most generic model describing spin-orbit-coupling effects is a two band model with a difference in Fermi velocities δv. This velocity difference destroys the spin-charge-separation and breaks the SU(2) symmetry in the low-energy Luttinger liquid theory. We show that electron-electron interactions then can open a gap in the spin sector of the theory when the interaction strength U is smaller than δv in appropriate units. The resulting spin-density-wave (SDW) state has a number of interesting properties reminiscent of topological insulators. We show that the the SDW state is robust against non-magnetic disorder and has zero-energy edge modes localized at its boundary.

TT 57: Transport: Fluctuations and Noise (jointly with CPP, DY)

Time: Wednesday 11:30–12:45 Location: H 3005

TT 57.1 Wed 11:30 H 3005

Quantum transport, master equations, and exchange fluctuations — •Sigmund Kohler and Robert Hussein — Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain

We investigate to which extent a many-body Bloch-Redfield master equation description of transport in coupled quantum dots is consistent with the exact generalized equilibrium conditions known as exchange fluctuation theorems. Thereby we identify a class of master equations for which this is the case. Beyond this class, we find deviations which exhibit characteristic scaling laws as functions of the dot-lead tunneling, the inter-dot tunneling, and the temperature. These deviations are accompanied by an increase of lead energy fluctuations inherent in the Bloch-Redfield equation beyond rotating-wave approximation. We illustrate our results with numerical data for a double and a quadruple quantum dot attached to four leads.

[1] R. Hussein and S. Kohler, Phys. Rev. B **89**, 205424 (2014).

TT 57.2 Wed 11:45 H 3005

Waiting time-distribution of a quantum-dot spin valve — •Björn Sothmann — Département de Physique Théorique, Université de Genève, Genève, Switzerland

Recently, the study of waiting-time distributions of electron transport has received a lot of interest [1]. It can provide information about transport processes that is complementary to average current and noise. Here, we discuss the waiting-time distribution of a a quantum-dot spin valve [2], i.e., a single-level quantum dot coupled to two ferromagnetic electrodes with magnetizations that can point in arbitrary directions [3]. We demonstrate that the rich transport physics of this setup, such as the dynamical channel blockade and spin precession in an interaction-driven exchange field, shows up in the waiting-time distribution, and we analyze the conditions necessary to observe the various effects.

[1] M. Albert, G. Haack, C. Flindt, M. Büttiker,
Phys. Rev. Lett. **108**, 186806 (2012).
[2] B. Sothmann, Phys. Rev. B **90**, 155315 (2014).
[3] M. Braun, J. König, J. Martinek,
Phys. Rev. B **70**, 195345 (2004).

TT 57.3 Wed 12:00 H 3005

Waiting-time distribution of light from superconducting resonators coupled to voltage-biased Josephson junctions — •Simon Dambach, Björn Kubala, Vera Gramich, and Joachim Ankerhold — Institute for Complex Quantum Systems, Ulm University, Ulm, Germany

The interplay of the tunneling transfer of charges and the emission and absorption of light can be investigated in a set-up, where a voltage-biased Josephson junction is placed in series to a microwave cavity. In such devices measurements of the emitted microwave radiation can yield information about the Cooper pair current and its fluctuations and vice versa.

Due to the inherent nonlinearity of the Josephson junction tunneling Cooper-pairs can create a variety of non-classical states of light already at weak driving. Depending on experimental parameters and tuning, the device can be described by effective Hamiltonians, indicating specific photon creation mechanisms which lead to strongly bunched or anti-bunched light emission [1].

We will use the waiting-time distribution [2] of emitted photons to highlight how charge quantization of the Cooper pair current drives a crossover from a coherent light source to a single-photon source. Analytical results for the weak driving regime, based on a quantum regression approach, are complemented by numerical results for the full nonlinear quantum case.

[1] B. Kubala, V. Gramich, and J. Ankerhold, arXiv:1404.6259.
[2] T. Brandes, Ann. Phys. (Berlin) **17**, 477 (2008).

TT 57.4 Wed 12:15 H 3005

Input-output description of microwave radiation in the dynamical Coulomb blockade — Juha Leppäkangas[1], Göran Johansson[1], •Michael Marthaler[2], and Mikael Fogelström[1] — [1]Microtechnology and Nanoscience, MC2, Chalmers Universit y of Technology, SE-412 96 Göteborg, Sweden — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany

We study microwave radiation emitted by a small voltage-biased Josephson junction connected to a superconducting transmission line. An input-output formalism for the radiation field is established, using a perturbation expansion in the junction's critical current. Using output field operators solved up to the second order, we estimate the spectral density and the second-order coherence of the emitted field. For typical transmission line impedances and at frequencies below the main emission peak at the Josephson frequency, radiation occurs predominantly due to two-photon emission. This emission is characterized by a high degree of photon bunching if detected symmetrically around half of the Josephson frequency. Strong phase fluctuations in the transmission line make related nonclassical phase-dependent amplitude correlations short lived, and there is no steady-state two-mode squeezing. However, the radiation is shown to violate the classical Cauchy-Schwarz inequality of intensity cross-correlations, demonstrating the nonclassicality of the photon pair production in this region.

TT 57.5 Wed 12:30 H 3005

Distribution of energy dissipated by a driven two-level system — •Philip Wollfarth[1,2], Alexander Shnirman[1,2], and Yasuhiro Utsumi[3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]Department of Physics Engineering, Faculty of Engineering, Mie University, Tsu, Mie, 514-8507, Japan

In the context of fluctuation relations, we study the distribution of energy dissipated by a driven two-level system. Incorporating an energy counting field into the well known spin-boson model enables us to calculate the distribution function of the amount of energy exchanged between the system and the bath. We also derive the conditional distribution functions of the energy exchanged with the bath for particular initial and/or final states of the two-level system. We confirm the symmetry of the conditional distribution function expected from the theory of fluctuation relations. We also find that the conditional distribution functions acquire considerable quantum corrections at times shorter or of the order of the dephasing time. Our findings can be tested using solid-state qubits.

[1] P. Wollfarth, A. Shnirman, Y. Utsumi,
Phys. Rev. B **90**, 165411 (2014).

TT 58: Spincaloric Transport I (jointly with MA)

Time: Wednesday 9:30–11:30 Location: H 0110

TT 58.1 Wed 9:30 H 0110

The Origin of spin Seebeck effect in Iron Garnet thin films — •Er-Jia Guo[1], Andreas Kehlberger[1], Gerhard Jakob[1], Matthias B. Jungfleisch[2], Burkard Hillebrands[2], Francesco D. Coletta[3], Hans Hübl[3], Stephan Geprägs[3], Sebastian Goennenwein[3], Rudolf Gross[3], and Mathias Kläui[1] — [1]Institute für Physics, Universität Mainz, 55099 Mainz, Germany — [2]Fachbereich Physik, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [3]Walther-Meißner-Institut, Garching, Germany

The discovery of spin Seebeck effect (SSE) provides an exciting approach to generate spin currents, which are suggested to replace charge currents in order to reduce the power dissipation. However, the genuine origin of SSE is still under debate. Here, we present thickness and temperature dependences of SSE signals in Yttrium Iron Garnet (YIG) and Gadolinium Iron Garnet (GIG) films. Using Pt/YIG hybrid structures, the thickness dependence of the material shows that magnonic spin currents are the source of the SSE.[1] We find a thickness-dependent enhancement of the SSE at low temperatures, which agrees well with the thermal conductivity, implying the importance of the magnon-phonon drag. In contrast to YIG, the GIG films allow us to measure the SSE across the compensation point.[2] Two sign changes of the SSE are observed with temperature drop, revealing the SSE is not simply mirroring to the total magnetization but the magnons emitted from three interacting magnetic sub-lattices as well as the spin-mixing conductances depending on the atom type at the interface.[1]A.Kehlberger,et al.,arXiv:1306.0784 (2013)[2]S.Geprägs,et al.,arXiv:1405.4971(2014)

TT 58.2 Wed 9:45 H 0110

High tunnel magneto-Seebeck effect — •Alexander Boehnke[1], Marvin von der Ehe[2], Christian Sterwerf[1], Christian Franz[3], Michael Czerner[3], Karsten Rott[1], Andy Thomas[1], Christian Heiliger[3], Markus Münzenberg[2], and Günter Reiss[1] — [1]CSMD, Physics Department, Bielefeld University, Germany — [2]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, Germany — [3]1. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany

Semiconducting materials are known to have large Seebeck coefficients. This is mainly attributed to the gap in their band structure and the asymmetric position of the Fermi-level with respect to this gap. Accordingly, half-metals with a band-gap for only one spin-channel may have very different Seebeck coefficients for the majority and minority charge carriers. The tunnel magneto-Seebeck effect (TMS) is a powerful tool to investigate such spin-dependent Seebeck coefficients because separate spin-channels can be defined in magnetic tunnel junctions (MTJs).

Here, we probe the spin-dependent Seebeck coefficients of half-metallic Heusler compounds in Heusler/MgO/CoFe MTJs. For Co_2FeSi we found a TMS ratio of 96%, which is much larger than that of CoFeB/MgO/CoFeB MTJs (4%). Furthermore, we found an increase in the mean Seebeck voltage from 30μV in CoFeB to 3mV in Co_2FeSi based MTJs, which agrees with *ab initio* calculations. We will explain these findings by a Julliere-like model, which also shows the importance of the asymmetric Fermi-level position.

TT 58.3 Wed 10:00 H 0110

How to control and determine the direction of thermal gradients in spin caloric measurements? — •Timo Kuschel, Tristan Matalla-Wagner, Michel Bovender, Oliver Reimer, Daniel Meier, Jan-Michael Schmalhorst und Günter Reiss — CSMD, Physics Department, Bielefeld University, Germany

In *longitudinal* spin Seebeck effect (LSSE) measurements in magnetic insulators like $NiFe_2O_4$ or $Y_3Fe_5O_{12}$ with an out-of-plane thermal gradient ∇T additional magnetic proximity effects in the adjacent spin detector material (e.g. Pt) have to be taken into account and can be identified or excluded by e.g. x-ray resonant magnetic reflectivity [1]. In *transverse* SSE experiments with in-plane ∇T unintended out-of-plane ∇T can induce additional contributions as mainly Nernst effects in magnetic metals [2] and primarily LSSE in magnetic insulators [3]. Therefore, the control and the determination of thermal gradient directions in spin Seebeck experiments should be investigated in detail. Here, we present a new spin caloric setup which allows the rotation of in-plane thermal gradients based on the vectorial superposition of $\nabla_x T$ and $\nabla_y T$. We check the in-plane direction of ∇T by an infrared camera and will use the setup to study established and new spin caloric effects for different ∇T directions. We further show exemplarily that linear and quadratic Nernst effects in CoFeTb thin films can be used to estimate the effective direction of ∇T in all three spatial directions.

[1] T. Kuschel et al., submitted 2014, arxiv: 1411.0113
[2] D. Meier et al., Phys. Rev. B 88, 184425 (2013)
[3] D. Meier et al., submitted 2014, arxiv: 1411.6790

TT 58.4 Wed 10:15 H 0110

Spincaloric properties of epitaxial $Co_2MnSi/MgO/Co_2MnSi$ magnetic tunnel junctions — •Benjamin Geisler and Peter Kratzer — Fakultät für Physik and Center for Nanointegration, Universität Duisburg-Essen, 47048 Duisburg, Germany

Magnetic tunnel junctions (MTJs) with ferromagnetic, half-metallic electrodes are interesting spintronics devices due to their high tunnel magnetoresistance ratio. If a thermal gradient is applied to such a MTJ, the relative electrode magnetization can be detected by measuring the induced voltage, i.e., by exploiting the magneto-Seebeck effect [Nat. Mater. 10, 472 (2011)].

Here we present an *ab initio* viewpoint on transport and spincaloric properties of epitaxial $Co_2MnSi/MgO(001)/Co_2MnSi$ MTJs. We compare results calculated with the conventional Sivan-Imry approach to results obtained from solving the Landauer-Büttiker equation directly. The latter procedure circumvents the linear response approximation inherent in the Seebeck coefficient and provides the response of the system (current or voltage) to arbitrary thermal gradients. Moreover, thermal variations of the chemical potential in the leads and finite-bias effects can be readily included in this method, but are found to be negligible for this specific MTJ. We show how the spincaloric properties of the MTJs depend on the interface atomic structure and that they can be tailored by a targeted growth control. Finally, we briefly comment on the perturbing influence of thermally activated electrode phonons and interface magnons on the tunneling transport.

TT 58.5 Wed 10:30 H 0110

Coherent spin wave scattering at defects and localization phenomena — •Martin Evers and Ulrich Nowak — University of Konstanz, 78457 Konstanz, Germany

From studies of transport of particles and waves it is known that there are different transport regimes. Under ideal conditions, like in vacuum or in a perfect crystal, transport will be ballistic. However, in reality one has usually to deal with some kind of imperfections that induce disorder in the system. If this disorder is strong enough the transport will become diffusive. As Anderson showed back in 1958 in case of phase coherent scattering disorder can also lead to completely suppressed transport, known as Anderson Localization [1]. For the case of spin waves this could lead to a vanishing magnon propagation length, even without any damping mechanism.

In the framework of a classical spin model the effect of disorder on magnonic transport is studied utilizing the Landau-Lifshitz-Gilbert equation. Numerical investigations of one and two dimensional systems give insight to scattering properties of the systems, e. g. the mean free scattering time. We show directly the existence of Anderson localization in 1D and weak localization, which is a precursor for strong localization, in 2D, showing the ubiquitousness of Anderson Localization in wave physics.

[1] P. W. Anderson, Phys. Rev. 109, 1492 (1958)

TT 58.6 Wed 10:45 H 0110

Spin-Phonon Interactions and Magnetoelastic Modes — •Matthias Assmann and Ulrich Nowak — University Konstanz, 78457 Konstanz, Germany

For modern spin-caloritronic applications in insulators the interactions between the magnonic and the phononic system play the decisive role. We developed a model, which allows a coupling between these two thermodynamic sub-systems under strict observance of energy and angular momentum conservation laws. For this model we perform spin-molecular dynamics simulations, which take into account the spatial as well as the spin degrees of freedom. The coupling between the spin and lattice degrees of freedom is achieved by pseudo dipolar forces. A temperature gradient is applied by appropriate boundary condition and the excitation of magneto-elastic modes in form of a coupled transport

of magnons and phonons in the temperature gradient is studied.

TT 58.7 Wed 11:00 H 0110

Anisotropic magnetothermopower in Co-based trilayers: A comparison between Cu, Pd, and Pt as heterostructure partners — •Voicu Popescu and Peter Kratzer — Faculty of Physics and CENIDE, University Duisburg-Essen, 47057 Duisburg, Germany

Within the framework of the spin-polarized relativistic Korringa-Kohn-Rostoker Green's function method we investigate the magnetothermopower (MTP) in a series of M/Co/M (M = Cu, Pd, and Pt) trilayer systems. As thermoelectric analogue of the conventional anisotropic magnetoresistance (AMR), the amplitude of the MTP signal is shown to depend on the asymmetry of the AMR around the Fermi energy. This asymmetry is sizable even if the magnetic layer itself displays only a small AMR, thus providing a path towards an efficient spin read-out thermoelectric device based on a single ferromagnetic layer. Our calculations establish a direct correlation between the strength of the spin-orbit coupling, modulated by the heterostructure partner M, and the MTP. The role of Co/M interface related effects such as structural relaxation and interdiffusion is also discussed.

TT 58.8 Wed 11:15 H 0110

Anisotropic magneto-thermopower in (Ga,Mn)As thin films — •Sibylle Meyer[1,2], Matthias Althammer[1], Wladimir Schoch[3], Rudolf Gross[1,2,4], and Sebastian T. B. Goennenwein[1,4] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, TU München, Garching, Germany — [3]Institut für Quantenmaterie, Universität Ulm, Ulm, Germany — [4]Nanosystems Initiative Munich, München, Germany

The resistance of ferromagnetic metals depends on the magnetization orientation. This is referred to as anisotropic magneto-resistance (AMR), and exploited in many applications. In close analogy, also the thermopower of magnetic metals depends on the magnetization orientation, i.e., the electrical field arising upon the application of a thermal gradient to the metal characteristically varies with the magnetization orientation (anisotropic magneto-thermopower AMTP). However, due to different symmetry restrictions, the evolution of AMR and AMTP with magnetization orientation is expected to be distinctly different. To experimentally test this conjecture, we measured the AMTP in (Ga,Mn)As single crystals. Our data show that the AMTP effect can be adequately modeled only if the symmetry of the (Ga,Mn)As crystal is explicitly taken into account. We quantitatively compare the AMTP with AMR data taken on the same (113)-oriented (Ga,Mn)As thin films and with corresponding model calculations.
Financial support by DFG via SPP 1538 is gratefully acknowledged.

TT 59: Multiferroics I (jointly with DF, DS, KR, MA)

Time: Wednesday 9:30–13:00 Location: EB 107

TT 59.1 Wed 9:30 EB 107

Magnetoelectric domain control in multiferroic $TbMnO_3$ — •Sebastian Manz[1], Masakazu Matsubara[1,2], Masahito Mochizuki[3,4], Teresa Kubacka[1], Ayato Iyama[5], Nadir Aliouane[6], Tsuyoshi Kimura[5], Steven Johnson[1], Dennis Meier[1], and Manfred Fiebig[1] — [1]ETH Zürich — [2]Tohoku University — [3]Aoyama Gakuin University — [4]Japan Science and Technology Agency — [5]Osaka University — [6]Paul Scherrer Institute

Spin-spiral multiferroics exhibit a strong coupling between the electric and magnetic subsystems which is of potential interest for technological applications. Although these systems have been investigated for more than a decade, the magnetoelectric domain evolution under external fields is still largely unknown. Using optical second harmonic generation we resolve how electric and magnetic fields affect the multiferroic domains in the archetypal spin-spiral multiferroic $TbMnO_3$. In consecutive electric switching cycles, varying multi-domain patterns emerge before a single-domain state is obtained. This observation reflects that the domain walls can easily move without being pinned by, e.g., structural defects. In striking contrast to the electric-field response, multi-domain patterns persist when the polarization direction is flopped by applied magnetic fields. Here, a uniform polarization rotation is observed within all domains, which incorporates a transformation of neutral into nominally charged domain walls. Our results are explained based on numerical Landau-Lifshitz-Gilbert simulations and provide first evidence for the scalability of macroscopic magnetoelectric properties onto the level of domains.

TT 59.2 Wed 9:45 EB 107

Critical behavior at the order-disorder transition in multiferroic $DyMnO_3$ — •Markus Schiebl, Alexey Shuvaev, Anna Pimenov, Graeme Eoin Johnstone, Uladzislau Dziom, and Andrei Pimenov — Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna Austria

We present the results of detailed dielectric investigations of the relaxation dynamics in $DyMnO_3$ multiferroic manganite. In addition to known domain wall relaxation a second strong mode is observed at low frequencies. We provide an experimental evidence that the new relaxation mode is coupled to the chirality switching of the spin cycloid.

We demonstrate that the relaxation dynamics in $DyMnO_3$ is typical for an order-disorder phase transition. Therefore, $DyMnO_3$ follows an order-disorder transition scenario implicating that a short range cycloidal order of Mn-spins exists above T_C. The results suggest that the paramagnetic sinusoidal phase should be explained as a dynamic equilibrium between the clockwise and counterclockwise cycloidal magnetic orders. The short range order in the paraelectric phase is transformed to a long range cycloid at the ferroelectric transition temperature.

TT 59.3 Wed 10:00 EB 107

Biquadratic and four-spin ring interactions in orthorhombic perovskite manganites — •Natalya Fedorova, Andrea Scaramucci, Claude Ederer, and Nicola A. Spaldin — ETH Zurich, Materials Theory, Wolfgang-Pauli-Strasse 27, CH-8093, Zurich, Switzerland

We use *ab initio* electronic structure calculations, based on DFT within the GGA+U approximation, to estimate the microscopic exchange interactions in the series of orthorhombic perovskite manganites (o-RMnO$_3$), in order to find a model Hamiltonian which can provide an accurate description of the magnetism in these materials. At low temperatures o-RMnO$_3$ with small radii of R cations (therefore, large octahedral tiltings) demonstrate a spiral or E-type antiferromagnetic orderings (E-AFM), which drive their multiferroic properties. Usually the establishment of such magnetic orderings is explained within the framework of a Heisenberg model with competing nearest-neighboring (NN) and next-nearest-neighboring exchange interactions. However, we find that the mapping the results of *ab initio* calculations onto the Heisenberg Hamiltonian for o-RMnO$_3$ show a clear deviation from the Heisenberg-like behavior. We demonstrate that this deviation can be explained only by the presence of biquadratic and four-spin ring exchange couplings and show that they have the strongest effect in compounds where NN exchange interactions are weakened, for example, due to large octahedral tiltings.

TT 59.4 Wed 10:15 EB 107

Time resolved polarized neutron scattering and dielectric spectroscopy reveal multiferroic domain dynamics in $MnWO_4$ and $TbMnO_3$ — •Jonas Stein[1], Daniel Niermann[1], Christoph Grams[1], Max Baum[1], Tobias Cronert[1], Jeannis Leist[2], Karin Schmalzl[3], A Agung Nugroho[4], Alexander C Komarek[5], Götz Eckold[2], Petra Becker[6], Ladislav Bohatý[6], Joachim Hemberger[1], and Markus Braden[1] — [1]II. Physikalisches Institut, Uni Köln — [2]Institut für Phys. Chemie, Uni Göttingen — [3]JCNS at ILL, France — [4]Institut Teknologi Bandung, Indonesia — [5]MPI Dresden — [6]Institut für Kristallographie, Uni Köln

Multiferroic materials are promising for future memory devices with low power consumption. The rise time between two states is a crucial parameter for a possible application and was investigated in the spin spiral multiferroics $TbMnO_3$ and $MnWO_4$. Polarized neutron diffraction is able to determine the ratio of chiral domains, which can be controlled by an electric field. Using the stroboscopic technique we follow the reversion of chiral domains in the timescale of a few hundred microseconds to hours. In $TbMnO_3$ we find a simple logarithmic relation between the rise time and temperature that is fulfilled over 5 decades. Broadband linear and nonlinear dielectric spectroscopy re-

vealed the domain dynamics in the MF phase of $MnWO_4$. The rise time reaches values in the minute range in the middle of the multiferroic temperature regime at T≈10 K but unexpectedly decays again on approaching the lower, first-order phase boundary at T_{N1}≈7.6 K.

[1] Niermann et al. **PRB 89**,134412 [2] Baum et al. **PRB 89**,144406

TT 59.5 Wed 10:30 EB 107

Polarization control at spin-driven ferroelectric domain walls — •Naëmi Leo[1], Anders Bergmann[2], Andres Cano[3], Narayan Poudel[4], Bernd Lorenz[4], Manfred Fiebig[1], and Dennis Meier[1] — [1]ETH Zurich, Switzerland — [2]Uppsala University, Sweden — [3]University Bordeaux, France — [4]University of Houston, USA

As was recently demonstrated, domain walls in ferroelectric materials show emergent electronic properties, like enhanced conductivity tunable by the relative orientation of the polarisation in the adjacent domains. Here, multiferroic materials with a coexistence of magnetic and electric order offer a new route for the control of such localised functionalities at domain boundaries.

Using spatially-resolved optical second harmonic generation we demonstrate the magneto-electric-field control of the multiferroic domains in Co-doped $MnWO_4$. In particular, the obtained domain distribution remains unchanged upon the magnetic-field-induced continuous 90°-rotation of the ferroelectric polarization.

This stability implies that multiferroic domain walls can accommodate for varying local polarisation configurations leading to local charging and discharging. We discuss the microscopic structure of the domain walls using micro-magnetic simulations.

TT 59.6 Wed 10:45 EB 107

Tuning order-by-disorder multiferroicity in CuO by doping — •Johan Hellsvik[1,2], Marcello Balestieri[1], Tomoyasu Usui[3], Alessandro Stroppa[2], Anders Bergman[4], Lars Bergqvist[5], Dharmalingam Prabhakaran[6], Olle Eriksson[4], Silvia Picozzi[2], Tsuyoshi Kimura[3], and José Lorenzana[1,2] — [1]ISC-CNR, Rome, Italy — [2]CNR-SPIN, L'Aquila, Italy — [3]Osaka University, Osaka, Japan — [4]Uppsala University, Uppsala, Sweden — [5]KTH, Stockholm, Sweden — [6]University of Oxford, Oxford, United Kingdom

The high Curie temperature multiferroic compound CuO has a quasidegenerate magnetic ground state that makes it prone to manipulation by the so-called "order-by-disorder" mechanism. First principle computations supplemented with Monte Carlo simulations and experiments show that isovalent doping allows us to stabilize the multiferroic phase in nonferroelectric regions of the pristine material phase diagram with experiments reaching a 250% widening of the ferroelectric temperature window with 5% of Zn doping. Our results allow us to validate the importance of a quasidegenerate ground state on promoting multiferroicity on CuO at high temperatures and open a path to the material engineering of multiferroic materials. In addition we present a complete explanation of the CuO phase diagram and a computation on the incommensurability in excellent agreement with experiment without free parameters.

[1] J. Hellsvik et al., Phys. Rev. B 90, 014437 (2014) [2] T. Kimura et al., Nature Mat. 7, 291 (2008) [3] G. Giovannetti et al., Phys. Rev. Lett. 106, 026401 (2011)

TT 59.7 Wed 11:00 EB 107

Dielectric properties and electrical switching behavior of the spin-driven multiferroic $LiCuVO_4$ — •Alexander Ruff[1], Stephan Krohns[1], Peter Lunkenheimer[1], Andrey Prokofiev[2], and Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Solid State Physics, Vienna University of Technology, Austria

The spin-1/2 chain cuprate $LiCuVO_4$ exhibits both ferroelectric and magnetic order at low temperatures. This so-called multiferroic behavior is of great scientific interest due to the underlying complex physical mechanisms, especially in the case of strong magnetoelectric coupling. Here we thoroughly discuss the multiferroic properties of the prototypical spin-driven ferroelectric material $LiCuVO_4$. At temperatures below about 2.5 K, it exhibits a three dimensional helical spiral spin order, with propagation in the *b* direction and a spin helix in the *ab* plane, which induces via an inverse Dzyaloshinskii-Moriya interaction a ferroelectric polarization in the *a* direction. In an external magnetic field, the direction of the spin spiral and thus the direction of the electrical polarization can be switched. This switching behavior of the polarization was demonstrated via dielectric spectroscopy on a single crystalline sample oriented in two different directions in magnetic fields up to 9 T. Detailed magnetic-field and temperature-dependent ferroelectric hysteresis-loop measurements imply the electric control of the spin helicity [1]. This rarely documented feature indicates the close coupling of electric and magnetic order of $LiCuVO_4$.

[1] A. Ruff *et al.*, *J. Phys.: Condens. Matter*, **26**:485901 (2014).

15 min coffee break

TT 59.8 Wed 11:30 EB 107

Emergence of ferroelectricity in multiferroic h-$YMnO_3$ — •Martin Lilienblum[1], Thomas Lottermoser[1], Sebastian Manz[1], Sverre M. Selbach[2], Andres Cano[3] und Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland — [2]Department of Material Science and Engineering, NTNU, N-7491 Trondheim, Norway — [3]CNRS, Université de Bordeaux, ICMCB, UPR 9048, F-33600 Pessac, France

Universal scaling laws, interfacial nano-electronics, and topological defects are currently studied using hexagonal manganites $R$$MnO_3$ (R= Sc, Y, Dy-Lu) as model system. In spite of the remarkably broad interest in the system, surprisingly little is known about the origin of the ferroelectric state. Here we solve the controversy about the emergence of the spontaneous polarization and its coupling to the underlying structural distortion by applying scanning probe microscopy (SPM) and optical second harmonic generation (SHG). We trace the spontaneous polarization by SHG from 100 K to 1450 K directly and contact-free. We find that only a single transition exists in which the polarization arises slower than expected as by-product of the structural distortion. By thermal treatments close to the structural transition and subsequent SPM scans, we show that the exceptionally robust ferroelectric domain pattern is determined only by the structural distortion. In summary we reveal that the ferroelectric order results from an interplay of electric polarization, topological effects, and temperature.

TT 59.9 Wed 11:45 EB 107

Monte Carlo approach to the ferroelectric phase transition in hexagonal manganites — •Thomas Lottermoser[1], Martin Lilienblum[1], Andres Cano[2], and Manfred Fiebig[1] — [1]ETH Zurich, Zurich, Switzerland — [2]Université de Bordeaux, Pessac, France

Despite several experimental and theoretical efforts in recent years the nature of the structural high temperature phase transition in the hexagonal manganites and its relation to the occurrence of a ferroelectric polarization in this materials is still not fully understood. Experimental data give two contradicting answers to this problem. Some experiments indicate a simultaneous appearance of the polarization in a single structural phase transition while others hint to a second phase transition several hundred Kelvin below the structural transition. In order to clarify these contradictions we performed Monte Carlo simulations based on the so-called clock model. In this model the six trimerization states of the manganite crystal structure are represented by six clock vectors in the complex plane. From the simulation data we calculated the temperature dependence of the complex structural order parameter and the induced ferroelectric polarization. The results point to a single phase transition with a strongly suppressed polarization contribution at high temperatures. This is experimentally confirmed by direct measurements of the ferroelectric polarization using optical second harmonic generation. Contradictions with other experimental data can be explained as finite size effects depending on the length scale of the experimental probe.

TT 59.10 Wed 12:00 EB 107

Magon-phonon interactions in hexagonal multiferroic $YMnO_3$ — •Andreas Kreisel[1], Shantanu Mukherjee[1], Brian M. Andersen[1], Turi Schäffer[1], Sonja Holm[1], Kim Lefmann[1], Niels C.R. Momsen[1], Jacob Larsen[2], Amy Fennell[3], Uwe Stuhr[3], and Zahra Yamani[4] — [1]Niels Bohr Institute, University of Copenhagen, Denmark — [2]Institute of Physics, Technical University of Denmark — [3]Laboratory of Neutron Scattering, Paul Scherrer Institute, Switzerland — [4]Chalk River National Laboratory, Canada

The multiferroic material $YMnO_3$ is known to show a large spin lattice coupling such that the spin and lattice degrees of freedom influence various properties, as for example the thermal conductivity that is found to have an anomalous contribution. The magnetoelastic modes have been measured recently in neutron diffraction experiments and linked to certain spectral features in Raman signals. Starting from a Heisenberg model on a triangular lattice with single ion anisotropies, we investigate the spin-phonon coupling via the magnetostriction mechanism

and derive a coupled magnon-phonon model valid in the entire Brillouin zone. Within a spin-wave approach, where the coupling yields a hybrid magnon-phonon mode, we calculate the dynamic structure factor and compare to recent experimental neutron results.

TT 59.11 Wed 12:15 EB 107

Stability of magnetic and electric domains against chemical doping in hexagonal manganites — •Ehsan Hassanpour Yesaghi, Viktor Wegmayr, Jakob Schaab, Dennis Meier, and Manfred Fiebig — Department of Materials, ETH Zürich, Zürich, Switzerland

The unique properties of magnetoelectric multiferroics are, to a large extent, determined by the coexistence and interaction of magnetic and electric domains. A major challenge towards future applications is to optimize the properties of these domains, such as their transport, without weakening or even losing the existing multiferroic order. Here, we present our study of ferroelectric and antiferromagnetic domains in chemically doped hexagonal manganites. We show that the electronic conductance of $ErMnO_3$ can be enhanced or suppressed by introducing either divalent (Ca^{2+}) or tetravalent (Zr^{4+}, Ti^{4+}) ions into the system. Using piezoresponse force microscopy (PFM) and optical second harmonic generation (SHG) we monitor the corresponding changes on the level of domains. We find that the $RMnO_3$-characteristic domain topography, as well as the multiferroic transition temperature, are robust against the applied ionic alteration, which demonstrates the usability of chemical doping for non-perturbative property-engineering of multiferroic domains.

TT 59.12 Wed 12:30 EB 107

Anisotropy study of multiferroicity in the pyroxene $NaFeGe_2O_6$ — •Lionel Andersen[1], Thomas Lorenz[1], Matthias Ackermann[2], Ladislav Bohatý[2], and Petra Becker[2] — [1]II. Physikalisches Institut - Universität zu Köln, Germany — [2]Institut für Kristallographie - Universität zu Köln, Germany

Since the mineral aegirine was found to be the first multiferroic member of the pyroxenes an intensive search for further related multiferroics was initiated [1]. In this contribution, we present a detailed study of the dielectric, magnetic and magnetoelastic properties of the pyroxene $NaFeGe_2O_6$ with special respect to the anisotropy. Unlike other investigations on $NaFeGe_2O_6$ [2] large single crystals where synthesized to examine pyroelectric currents, dielectric constants and magnetic susceptibilities as well as the thermal expansion and the magnetostriction. The spontaneous electric polarization detected below $T_C \simeq 11.6$ K in an antiferromagnetically ordered state ($T_N \simeq 13$ K) is mainly lying within the *ac* plane with a small component along *b*, indicating a triclinic symmetry of the multiferroic phase of $NaFeGe_2O_6$. The electric polarization can be strongly modified by applying magnetic fields along different directions. We derive detailed magnetic-field versus temperature phase diagrams and identify three multiferroic low-temperature phases, which are separated by a non-ferroelectric, antiferromagnetically ordered state from the paramagnetic high-temperature phase [3].

[1] S. Jodlauk *et al.* J. Phys.: Condens. Matter **19** (2007)
[2] I. Kim *et al.* J. Phys.: Condens. Matter **24** (2012)
[3] M. Ackermann *et al.* New J. Phys. (submitted, arXiv:1408.6772)

TT 59.13 Wed 12:45 EB 107

***Ab Initio* analysis of ferroelectric and magnetic properties of potentially multiferroic aurivillius phases** — •Axiel Yael Birenbaum, Jan van den Broek, and Claude Ederer — Materials Theory, ETH Zürich

A promising class of high temperature polar magnetic multiferroic materials are the Aurivillius family of layered-perovskites related compounds. They combine high temperature ferroelectric properties with a layered structure that allows for systematic introduction of magnetic ions. The simplest of such cases to have been studied is $Bi_5FeTi_3O_{15}$. However, no well-established value exists for its spontaneous electric polarization, and contradictory reports as to its magnetic states.

We perform Density Functional Theory calculations on $Bi_5FeTi_3O_{15}$, and conclude on a high spontaneous electric polarization. To better understand the mechanism for ferroelectricity, we examine 9 systems, based on $SrBi_2Ta_2O_9$ as reference. We find a high spontaneous polarization even in the case of with no nominally ferroelectrically-active cations. We discuss these results in light of the tri-linear coupling between soft and hard modes demonstrated for $SrBi_2Ta_2O_9$ and the general concept of "hybrid improper ferroelectricity". To clarify the range of temperatures expected for magnetic long range order despite a low concentration of magnetic ions and the short range of superexchange interactions, we perform Monte Carlo simulations. We discuss possible strategies to increase magnetic ordering temperatures.

TT 60: Organic Electronics and Photovoltaics: OPV II (jointly with CPP, HL)

Time: Wednesday 9:30–13:00 Location: C 130

TT 60.1 Wed 9:30 C 130

Impact of Mesoscale Order on Energetics in Organic Semiconductors — •Carl Poelking[1], Max Tietze[2], Chris Elschner[2], Selina Olthof[3], Dirk Hertel[3], Björn Baumeier[1], Frank Würthner[4], Klaus Meerholz[3], Karl Leo[2], and Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institut für Angewandte Photophysik, Dresden, Germany — [3]Physikalische Chemie, Universität zu Köln, Germany — [4]Institut für Organische Chemie, Universität Würzburg, Germany

The interaction of charged excitations with the molecular surrounding in organic semiconductors is strictly long-ranged, due to their quadrupolar building blocks and preferential or absolute structural order. We show how atomistic simulations access the resulting energetics of charges and charge pairs and derived quantities, notably the charge-density-dependent open-circuit voltage across organic heterojunctions, with excellent accuracy. We compute level diagrams for a variety of donor-fullerene interfaces, with direct experimental validation. The underlying simulation approach takes into account long-range electrostatic effects that persist up to the mesoscale. The resulting mesoscale fields not only produce flat level profiles, but provide orientation-dependent push-out forces across a donor-acceptor interphase that can drive the charge-separation process. Correct polarity of these push-out forces is a requirement for functional solar cells, with operation closely above an isopolar point as the optimum tradeoff between magnitude of these push-out forces and the photovoltaic gap.

TT 60.2 Wed 9:45 C 130

Signature of the Dirac cone in the excitation gaps of linear oligoacenes — •Richard Korytár — Institut für Nanotechnologie, Karlsruher Institut für Technologie, Herrmann-von-Helmholtzplatz 1, 76344 Eggenstein-Leopoldshafen

Linear oligoacenes (linearly fused benzene rings) are one of the prototypical examples of quantum wires and the simplest realization of the so called nano-graphene. We show that contrary to a widely held belief, the excitation gaps of oligoacenes can display oscillations of period 11 (rings) as a function of the molecule's length. By inspection of the polyacene electronic band-structure, we show that the incommensurate oscillations are caused by the presence of an accidental degeneracy at the Fermi level, reminiscent to the Dirac cone of graphene. Our predictions are supported by calculations based on density functional theory. We clarify the role of interactions by studying a parameterized Hubbard model with density matrix renormalization group. Our findings may have implications for organic electronics and research of materials for energy conversion.

TT 60.3 Wed 10:00 C 130

Probing Interfacial Properties in Polymer:Fullerene Bulk Heterojunctions — •Christian Kästner[1], Daniel A. M. Egbe[2], and Harald Hoppe[1] — [1]Institute of Physics, Technische Universität Ilmenau, Ilmenau, Germany — [2]Linz Institute for Organic Solar Cells, Johannes Kepler University, Linz, Austria

We investigated the properties of donor-acceptor interfaces occurring in fine-tuned ternary bulk heterojunctions and were able to quantitatively correlate spectroscopic information with domain phase order. Relaxation energies for AnE-PV donor polymers as well as of PCBM were found to range within 100-200 meV.

TT 60.4 Wed 10:15 C 130

The Effect of Solvent Additive on Generation, Recombination and Extraction in PTB7:PCBM Solar Cells: A conclusive Experimental and Numerical Simulation Study — •Juliane Kniepert[1], Ilja Lange[1], Thomas Brenner[1], Jan Anton Koster[2], and Dieter Neher[1] — [1]Universität Potsdam, Germany — [2]University of Groningen, The Netherlands

Time delayed collection field (TDCF), bias amplified charge extraction (BACE) and space charge limited current (SCLC) measurements are combined with complete numerical device simulations to unveil the effect of the solvent additive 1,8-diiodooctane (DIO) on the performance of PTB7:PCBM bulk heterojunction solar cells. DIO is shown to increase the charge generation rate, reduce geminate and bimolecular recombination and increase the electron mobility. In total, the reduction of loss currents by processing with the additive raises the power conversion efficiency of the PTB7:PCBM blend by a factor of almost three. Our device simulations show unambiguously that the effect of the additive on the shape of the current-voltage curve cannot be ascribed to the variation of only the mobility, the recombination or the field-dependence of generation. It is only when the changes of all three parameters are taken into account that the simulation matches the experimental J-V-characteristics under all illumination conditions and for a wide range of voltages.

TT 60.5 Wed 10:30 C 130

Quantification of loss channels in bulk heterojunction organic solar cells based on DPP-type donor-acceptor copolymers blended with PC71BM — •Julian Robert Ochsmann[1], Deepak Chandran[2,3], Kwang-Sup Lee[3], and Frédéric Laquai[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Dublin City University, Dublin, Ireland — [3]Hannam University, Daejeon, South Korea

A promising approach to improve the performance of bulk-heterojunction (BHJ) organic solar cells (OSC) is to use low-bandgap polymers as electron donor materials as they enhance the photon absorption of the photoactive layer in the near infrared wavelength range and thereby increase the photocurrent. In addition, low-bandgap polymers are suitable for use in tandem solar cells, since their absorption spectrum is complementary to that of mid-bandgap polymers such as P3HT or PCDTBT, which allows for photocurrent matching of front and back cells. A promising class of low-bandgap polymers for single- and multijunction solar cells are donor-acceptor type copolymers based on diketopyrrolopyrrole (DPP) units. In this study we investigate the photovoltaic performance and the photophysics of two DPP-based copolymers, namely PTDPP-TT and PFDPP-TT, blended with PC71BM and applied in single junction BHJ solar cells. The photophysics of the OSC devices were investigated with broadband transient absorption pump-probe spectroscopy (TA) and analyzed with a previously reported model of charge recombination that allows to quantify the loss channels in devices.

TT 60.6 Wed 10:45 C 130

Efficiency-Limiting Processes in Low-Bandgap Polymer:Perylene Diimide Photovoltaic Blends — •Dominik Gehrig[1], Steffen Roland[2], Ian Howard[1], Dieter Neher[2], and Frédéric Laquai[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz — [2]Institut für Physik und Astronomie, Physik weicher Materie, Universität Potsdam

In this work, we present a photophysical study on blends of a low-bandgap polymer, namely PBDTTT-C, as donor in combination with a PDI-based electron acceptor.[1] Exciton and charge carrier dynamics as well as loss mechanisms are investigated by sub-picosecond to microsecond pump-probe transient absorption (TA) and time-resolved photoluminescence (TRPL) spectroscopy in combination with multivariate curve resolution (MCR) data analysis. A largely diffusion-limited exciton dissociation at the donor acceptor interface and consequently a slow charge generation is observed. Time-delayed collection field (TDCF) experiments reveal a strongly field-dependent charge generation process in turn leading to low fill factors in devices. However, once free charges are generated they recombine non-geminately on a ns-us timescale indicating that they can be potentially extracted as photocurrent. By comparison of the PBDTTT-C:PDI charge generation efficiency with that of a PBDTTT-C:fullerene blend, we identify inefficient charge generation and fast non-geminate recombination competing with charge extraction to be the main bottlenecks of photocurrent generation in the investigated polymer:PDI blends.

[1] Gehrig et al., J. Phys. Chem. C 2014, 118, 20077

TT 60.7 Wed 11:00 C 130

Effect of solvent vapor annealing on perylene-based solar cells — •Stefan Grob[1], Mark Gruber[1], Andrew Bartynski[2], Theresa Linderl[1], Mark Thompson[2], and Wolfgang Brütting[1] — [1]University of Augsburg, Augsburg, Germany — [2]University of Southern California, Los Angeles, USA

Diindenoperylene (DIP) and Tetraphenyldibenzoperiflanthene (DBP) are two common materials used in organic solar cell devices. While DIP is growing crystalline, showing good charge and exciton transport but only weak absorption, DBP exhibits an amorphous character, leading to lower carrier mobility and a short exciton diffusion length, however, DBP reveals a distinctly higher absorption. For both materials we investigate the influence of solvent vapor annealing (SVA) on solar cell performance. In general, SVA leads to a reorganization of the treated materials due to a partial re-solubilization of the layers, allowing the molecules to rearrange into structures characterized by a higher degree of order [1]. Though, for DBP, extended annealing times lead to a strong aggregation of the molecules, resulting in inhomogeneous layers unfavorable for solar cells. For DIP cells however, SVA leads to an increase in fill factor (FF) and also a slight increase in short-circuit current density (Jsc) due to interface roughening. Nevertheless, the best results are obtained by combining annealed DIP layers with strongly absorbing DBP and C70 on top. Thereby, we obtain the same increase in FF but a higher gain in Jsc, elevating the power conversion efficiency by almost 20 % up to more than 4 %.

[1] G. De Luca et al., J. Mater. Chem., 2010, 20, 2493-2498

15 min. break

TT 60.8 Wed 11:30 C 130

Morphology Tuning by Side-chain Variation in Bulk-Hetero-Junction Solar Cells Based on Merocyanines — •Dirk Hertel, Julian Nowak, Stephanie Rüth, Ruth Bruker, Jürgen Schelter, and Klaus Meerholz — Universität zu Köln, Department Chemie, Luxemburgerstrasse 116, 50939 Köln

Organic photovoltaics (OPV) offers the potential of mass-produced renewable energy. Within the last decade the efficiency of organic solar cells has increased from 3 % to 10 %, mainly based on better understanding and control of morphology. We investigate merocyanines (MC), a class of low-molecular-weight colorants, as donor material in organic solar cells. These molecules are processable via both deposition techniques showing remarkable power conversion efficiencies (PCE) beyond 4% for SOL- and 6% for VAC-processed devices. Despite these impressive numbers the understanding of the influence of morphology on charge generation, transport and recombination in MCs is in its infancy. To aim towards even higher PCEs we have systematically varied the side-chain of a prototypical donor-acceptor MC with a high ground state dipole moment. By applying atomic-force mircroscopy, transmission electron microscopy and x-ray diffraction we are able to elucidate the thin film structure and show how side-chain variation reduces domain size and improves device data. We are able to correlate crystal size to optical, morphological and device data. There is an optimum side chain length and contrary to previous observations the MC:PCBM blend layers processed from solution perform better in OPVs than layers processed by thermal deposition under vacuum.

TT 60.9 Wed 11:45 C 130

Exploring the performance enhancement potential of the tapering technology for block-copolymer solar cells using a novel particle-based multiscale solar-cell algorithm — Anton Pershin, Sergii Donets, and •Stephan Baeurle — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93040 Regensburg, Deutschland

Tapered block copolymers offer an exciting opportunity to tailor the interfacial region between different components by conserving their phase-separated mesoscale structure, which enable the generation of polymer systems with the desired spatio-dynamic properties. In this presentation, we explore their usefulness for optimizing the photovoltaic performance of polymer bulk heterojunctions. To this end, we apply a recently developed particle-based multiscale solar-cell algorithm [1,2] and investigate the effect of random tapering at the chemical junctions between the electron-donor- (D) and electron-acceptor-(A) blocks on the photovoltaic properties of various lamellar-like polyfluorene-based block-copolymer systems. Our simulation results [2] reveal that introducing a tapered middle block with optimal length leads to a significant increase of the exciton dissociation efficiency, but

deteriorates the charge transport efficiency only moderately. This results in a gain of the internal quantum efficiency from 25 up to 39 % by increasing the thickness of the active layer of the solar cell from 10 up to 50 nm in direction to the DA interface. Literature: [1] A. Pershin, S. Donets, S.A. Baeurle, Polymer 55, 3736 (2014); [2] A. Pershin, S. Donets, S.A. Baeurle, Polymer 55, 1507 (2014).

TT 60.10 Wed 12:00 C 130

Effect of alcohol treatment on the morphology and performance of PTB7:PC71BM bulk heterojunction solar cells — Shuai Guo[1], Biye Cao[1], Weijia Wang[1], Jean-Francois Moulin[2], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]Helmholtz-Zentrum Geesthacht am MLZ, Lichtenbergstr. 1, 85747 Garching

The environmentally friendly alcohol treatment of bulk heterojunction (BHJ) polymer solar cells using the low bandgap copolymer based on thieno[3,4-b]thiophene-alt-benzodithiophene units (PTB7) and [6,6]-phenyl-C71-butyric acid methyl ester (PC71BM) is studied. Different alcohols are tested and besides the most commonly used methanol treatment, other alcohols such as ethanol, 2-propanol, and 1-butanol also improve the device performance as compared to untreated solar cells. Changes of the surface structure caused by the alcohol treatment are probed with AFM and the modification of inner film morphology is probed by time of flight-grazing incidence small angle neutron scattering (TOF-GISANS). UV/Vis measurements show that the thickness of all BHJ films remains unchanged by the different solvent treatments. Thus, the enhanced device performance induced by the alcohol treatments is correlated to the reconstruction of the inner film structures probed with TOF-GISANS and the modified energy levels at the interfaces between the BHJ layer and the aluminum electrodes, evident by the enhanced short-circuit current and open-circuit voltage of the I-V curves.

TT 60.11 Wed 12:15 C 130

Control of Structural Order and Phase Separation in Polymer-Fullerene Solar Cells — •Christian Kästner[1], Daniel A. M. Egbe[2], and Harald Hoppe[1] — [1]Institute of Physics, Technische Universität Ilmenau, Ilmenau, Germany — [2]Linz Institute for Organic Solar Cells, Johannes Kepler University, Linz, Austria

It is common knowledge that polymer aggregation and phase separation in blends with fullerene derivatives is a delicate issue and crucially impacts the photovoltaic parameters of polymer based solar cells. On the one side, strongly intermixed polymer:fullerene phases provide large interfacial area and consequently large exciton dissociation rates and thus charge carrier generation. On the other side, pristine, and eligibly ordered, polymer or fullerene domains support exciton delocalization and efficient charge transport. Herein, we present versatile routes to control the morphology by applying side-chain modifications to the polymer and fullerene, tuning the polymer:fullerene blend ratio and controlling the order within the bulk heterojunction via ternary blends. On the basis of an anthracene-containing poly(p-phenylene-ethynylene)-alt-poly(p-phenylene-vinylene) (PPE-PPV) copolymer backbone we investigated a number of these structure-property-relations. As an imposing result it is demonstrated that via manipulation of molecular structure and processing parameters enables tuning bulk morphologies at will.

TT 60.12 Wed 12:30 C 130

Influence of post-production thermal stress on organic photovoltaic cells — •Arne Hendel, Marlis Ortel, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

One of the mayor challenges of organic photovoltaic cells towards large scale industrial production is the lifetime of the organic solar cells. Accelerated lifetime tests can be performed by applying thermal stress to the devices. In this study, PTB7:PCBM bulk hetero-junction solar cells were exposed in a post-production thermal heat step to temperatures up to 140°C. The reaction to thermal stress was investigated by impedance analysis and light intensity dependent I-V characteristics. It was found that the overall conductivity improved by thermal stress. In addition, an asymmetric series resistance which depends strongly on the light intensity was found by the light intensity dependent measurements. Furthermore, an investigation of the diode characteristic in dark revealed a deterioration of the blocking behaviour for reverse voltages. The results of the impedance analysis and light intensity dependent measurements were compared to AM1.5G I-V characterization, which was used to monitor the degradation of the device performance. A physical device model including the contact properties of the solar cells is presented to explain the findings.

TT 60.13 Wed 12:45 C 130

How intrinsic photo-degradation impacts photovoltaic device performance in organic solar cells — •Thomas Heumueller[1], Timothy Burke[2], William Mateker[2], Michael McGehee[2], and Christoph Brabec[1,3] — [1]Universität Erlangen-Nürnberg — [2]Stanford University — [3]ZAE Bayern

As organic PV efficiencies exceed 10%, the science of stabilization and lifetime gains importance. Several degradation phenomena in organic solar cells are related to an increase in trap density, but the mechanisms of how different types of traps affect open-circuit voltage, short-circuit current and fill factor need considerably more investigation. To separate effects from several different degradation mechanisms that usually occur at the same time, we perform tests under controlled environmental conditions and distinguish between bulk and interface effects by de-laminating and replacing electrodes. Interfacial degradation is observed to predominantly affect the fill factor, most likely due to the formation of energetic barriers and can be reversed by reapplying new electrodes. Bulk degradation in amorphous systems, like PCDTBT, results in a loss of open circuit voltage. Using charge extraction and transient photovoltage we show that the Voc losses are not caused by increased recombination, but rather by a broadening in the density of states. Crystalline materials demonstrate an increased stability against Voc losses, most likely due to a high charge carrier density at Voc. Sometimes a characteristic loss of short circuit current is observed in crystalline materials. We show that those losses can be prevented by choosing a different acceptor material.

TT 61: Frontiers of Electronic Structure Theory: Organics and Materials (jointly with O, HL)

Time: Wednesday 10:30–13:30 Location: MA 004

Invited Talk TT 61.1 Wed 10:30 MA 004

Transport and excitations in biased nano-junctions: DFT-based simulations — •Mads Brandbyge — Dept. of Micro and Nanotechnology, DTU-Nanotech, and Center for Nanostructured Graphene (CNG) Technical University of Denmark, Build. 345 east, 2800 Kongens Lyngby, DENMARK

In nano-junctions the electronic current is forced through a bottleneck down to the single molecular or atomic level. The highly non-equilibrium electronic system in such junctions results in various excitations such as phonons or plasmons. The phonon interaction directly yield signals in the current which can be probed in current-voltage spectroscopy, while the plasmon interaction can result in light emission which seems to be related to the current fluctuations/noise at finite frequency. The low frequency shot noise can provide information about the elastic transport channels and underlying spin-dependent electronic structure of the junctions. We will discuss how theory based on non-equilibrium Greens functions in combination with density functional theory or beyond, can be compared to experimental results, and provide important insights into excitations, the underlying transport channels, and electronic structure of the junctions. The electronic current will not only excite phonons. Energy non-conserving current-induced forces may control the resulting heat flow and heat distribution in the junctions, and in some cases lead to a break-down of the harmonic approximation.

TT 61.2 Wed 11:00 MA 004

Role of atomic multiplets in intermediate valence SmB_6 and PuB_6 systems — •Alexander B. Shick[1], Alexander I. Lichtenstein[2], and Mikhail I. Katsnelson[3] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [2]Institute of Theoretical Physics, University of Hamburg,

Hamburg, Germany — [3]Radboud University Nijmegen, The Netherlands

The materials with strong electron correlations are important because of the fundamental properties, and the technological applications. Recently, SmB_6 (as well as PuB_6) was proposed as 3D topological insulator [1]. The electronic structure calculations are performed combining the LDA with an exact diagonalization of the Anderson impurity model [2] for [Sm,Pu]B_6. For the Sm atom in SmB_6, intermediate valence ground state (GS) is found with the f-shell occupation $\langle n_{4f}\rangle = 5.6$. The GS is a singlet, and the first excited triplet state ~ 3 meV higher in the energy. The f-orbital density of states is in agreement with experimental PE spectra. SmB_6 is a narrow band insulator already in LDA, with the direct band gap of ~ 10 meV. The electron correlations increase the band gap which now becomes indirect. For the Pu atom in PuB_6, we also find intermediate valence ($\langle n_{5f}\rangle = 5.5$) singlet GS. The calculations illustrate that many-body effects are relevant to form the indirect band gap, and support the idea of "topological Kondo insulator" in SmB_6. [1] M. Dzero *et al.*, Phys. Rev. Lett. **104**, 106408 (2010); [2] A. B. Shick *et al.*, Phys. Rev. B **87**, 020505(R) (2013).

TT 61.3 Wed 11:15 MA 004

Transition paths and cohesive energies in alpha-sexithiophene polymorphs — •Bernhard Klett, Caterina Cocchi, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Like many organic crystals, oligothiophenes display polymorphism. Different molecular orientations and stacking arrangements are known to influence electronic and transport properties. An in-depth theoretical understanding of the energetics in these systems is crucial to control their growth and fully exploit their potential. In fact, their outstanding opto-electronic features make oligothiophenes excellent candidates for a number of technological applications, ranging from thin-film transistors to photovoltaic cells. We investigate alpha-sexithiophene in view of the transition between the high-temperature (HT) and low-temperature (LT) phase. With the full-potential all-electron density-functional theory code exciting [1], we analyse the cohesive properties of the two polymorphs. Our results indicate HT as the most stable phase, in agreement with previous molecular-dynamics simulations [2]. We also explore a transition path between the two polymorphs, suggesting different reaction coordinates. Our findings allow for estimating the energy barrier between the two phases, hence gaining insight into the microscopic mechanisms ruling polymorphism in organic crystals. [1] A. Gulans, et al., J. Phys.: Condens. Matter 26, 363202 (2014). [2] R. G. Della Valle, et al., J. Phys. Chem. A, 112, 6715 (2008).

TT 61.4 Wed 11:30 MA 004

Importance of the reorganization energy barrier in computational design of porphyrin-based solar cells with cobalt-based redox mediators — •Kristian Baruël Ørnsø, Elvar Örn Jónsson, Juan Maria Garcia-Lastra, Karsten Wedel Jacobsen, and Kristian Sommer Thygesen — Center for Atomic-scale Materials Design, Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

The shift from iodide based redox mediators in dye sensitized solar cells towards octahedral cobalt complexes has lead to a significant increase in the efficiency. However, due to the nature of this type of complexes the driving force required for the regeneration of the dye is very high and this limits the achievable efficiency. Here we show that the large driving force is a direct consequence of the large reorganization energy of the dye regeneration reaction. The reorganization energies for charge transfer between a simple zinc porphyrin dye and two popular cobalt based redox mediators is calculated using ab-initio molecular dynamics with explicit solvent. These results are then combined with a Marcus based extrapolation scheme to obtain the reorganization energies of more than five thousand porphyrin based dyes.We propose a scheme for scoring the performance of the porphyrin dyes which is able to identify already known high-performance dyes in addition to a number of even better candidates. Our analysis shows that large internal reorganization energy of the Co-based redox mediators is a main bottleneck for achieving higher efficiencies.

TT 61.5 Wed 11:45 MA 004

Ab initio Simulation of Optical Limiting: The Case of Metal-Free Phthalocyanine — •Caterina Cocchi[1,2], Deborah Prezzi[2], Alice Ruini[2,3], Elisa Molinari[2,3], and Carlo Andrea Rozzi[2] — [1]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [2]Centro S3, CNR Istituto-Nanoscienze, Modena, Italy — [3]Dipartimento di Scienze Fisiche, Informatiche, Matematiche, University of Modena and Reggio Emilia, Italy

Optical limiting (OL) is a nonlinear process that is relevant for an entire class of devices related to the protection of light-sensitive elements, including the human eye, from intense light sources. While extensively studied experimentally, an accurate theoretical investigation of this phenomenon is still missing. In the framework of time-dependent density-functional theory, we present a fully ab initio, non-perturbative description of OL properties of a metal-free phthalocyanine, a prototypical macrocyclic organic compound. By applying a broadband electric field of increasing intensity, we confirm that reverse saturable absorption is the leading mechanism for OL phenomena in this class of systems, and reveal that a number of dipole-forbidden excitations are populated by excited-state absorption at more intense external fields. The excellent agreement with the available experimental data supports our approach as an effective and powerful tool to describe and predict OL [1]. [1] C. Cocchi et al., Phys. Rev. Lett. 112, 198303 (2014).

TT 61.6 Wed 12:00 MA 004

High-throughput Screening of Perovskite Oxides and Related Compounds for Light Harvesting Applications — •Ivano E. Castelli[1], Nicola Marzari[1], Kristian S. Thygesen[2], and Karsten W. Jacobsen[2] — [1]Theory and Simulation of Materials, and EPFL National Center for Computational Design and Discovery of Novel Materials (MARVEL), EPFL, Lausanne, Switzerland — [2]Center for Atomic-scale Materials Design, Technical University of Denmark, Kgs. Lyngby, Denmark

Solar energy harvesting in a photoelectrochemical (PEC) cell, where water is split into hydrogen and oxygen, is an attractive and renewable contribution to our global needs of increasing energy demand and storage. We explore the possibility of identifying novel photocatalysts for PECs with the use of high-throughput quantum mechanical simulations. We devise inexpensive approaches to calculate systematically the structural and electronic properties of 19000 cubic ABX3 perovskites, obtained by combining 52 possible metals as A- or B-cations, together with oxygen, nitrogen, sulfur and fluorine as anions. Using the screening criteria of stability and bandgap, 20 promising materials have been identified for visible-light harvesting [1]. The problem of corrosion has been addressed, determining the Pourbaix diagrams of the candidates through a combination of experimental and computational data [2]. We also suggest a handful of lower symmetry layered and rare-earth perovskites for further theoretical and experimental investigation. References: [1] I. E. Castelli et al., Energy Environ. Sci. 5, 9034 (2012). [2] I. E. Castelli et al., Topics in Catalysis 57, 265 (2014).

TT 61.7 Wed 12:15 MA 004

Understanding and designing novel materials for energy — •Silvana Botti — Friedrich-Schiller-Universität Jena, Germany

I will present an overview of our most recent theoretical/computational developments and some examples of their application to calculate from first-principles the structural and electronic properties of materials for energy production, storage, and saving.

The systems we are interested in are varied, ranging from thin-films absorbers and transparent conductive oxides for solar cells, to thermoelectrics, light-weight materials for constructions, complex hydrides for on-board hydrogen storage.

Nowadays, ab initio approaches based on density functional theory ally accuracy and efficiency, which make them suitable for understanding the physics not only of simple bulk crystals, but also of nanostructures, crystals with defects, doped crystals, interfaces, alloys, etc. As a consequence, ab initio calculations are finally able to analyze the "real" samples measured in experiments, allowing accurate comparisons of both ground-state and excited-state properties.

Moreover, ab initio methods can be used together with structural prediction algorithms and evolutionary algorithms to solve the inverse problem, i.e. find the best material for a specific application, providing a precious guide for experimental search of novel materials.

TT 61.8 Wed 12:30 MA 004

Accurate density-functional theory calculation of bulk properties of 65 elemental solids — •Sven Lubeck[1], Andris Gulans[1,2], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Density-functional theory (DFT) is a common method for calculating various properties of molecules and solids. While a large part of errors in DFT calculations stems from approximations to the exchange-correlation functional, there are additional not well controlled errors introduced by numerical implementation of electronic structure codes. In this work, we present accurate benchmark calculations of equation of state for 65 non-magnetic elemental solids. The data have been obtained using the full-potential augmented-plane-waves (APW) code `exciting` [1]. High accuracy has been achieved by constructing a converged APW+lo basis set, which yields consistent bulk properties of considered solids for a range of augmentation sphere sizes. Using methodology suggested in Ref. [2], we compare our results to those obtained with WIEN2k [2] and find the average and maximum Δ-values of 0.3 meV/atom and 2.1 meV/atom, respectively.

[1] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, and C. Draxl, J. Phys.: Condens. Matter 26, 363202 (2014).
[2] K. Lejaeghere, V. Van Speybroeck, G. Van Oost and S. Cottenier, Critical Reviews in Solid State and Materials Sciences 39, 1-24 (2014).

TT 61.9 Wed 12:45 MA 004

Electronic phase transitions of bismuth under strain from relativistic self-consistent *GW* calculations — Irene Aguilera, •Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present quasiparticle self-consistent *GW* (QS*GW*) calculations of semimetallic bulk Bi. We go beyond the conventional QS*GW* method by including the spin-orbit coupling throughout the self-consistency cycle. This approach improves the description of the electron and the hole pockets considerably with respect to standard density functional theory (DFT), leading to excellent agreement with experiment. We employ this relativistic QS*GW* approach to conduct a study of the semimetal-to-semiconductor and the trivial-to-topological transitions that Bi experiences under strain. While DFT predicts that an unphysically large strain is needed for such transitions, we show that the relativistic QS*GW* description of the electronic structure moves the required strain into a regime that is likely to be realizable in experiment.
We acknowledge financial support from the Alexander von Humboldt Foundation and from the Helmholtz Association through the Virtual Institute for Topological Insulators (VITI).

TT 61.10 Wed 13:00 MA 004

A GW algorithm of reduced complexity for organic crystals — •Saber Gueddida[1], Dietrich Foerster[1], Peter Koval[2], and Daniel Sanchez-Portal[2] — [1]Laboratoire Ondes et Matière d'Aquitaine, University of Bordeaux, France — [2]Donostia International Physics Center, San Sebastian, Spain

Density functional theory (DFT) provides a variational estimate of the electronic structure and geometry of many materials in their ground state. By its construction, DFT is unsuited for a description of the excited states, and particularly so for semi conductors. For these, one resorts to Hedin's GW approximation that gives rather good bands and gaps. A practical limitation of this approach is its computational cost that increases with the fourth power (N**4) of the number of atoms N per unit cell. Starting in 2007 [1], we have developed methods of "reduced complexity" that lower the growth of CPU time in calculations of electronic structure from N**4 to N**3, both for optical absorption [2] and in the GW approximation for finite systems [3]. Here we report on the extension of our methods to crystals, where we reduce the growth of CPU time again from N**4 to N**3, with N now the number of atoms in the unit cell of the crystal. Our work is motivated by organic semiconductors that have too many atoms in their unit cell for O(N**4) algorithms to be practical. Our results should help to improve and optimize organic solar cells. [1] D. Foerster, J. Chem. Phys. 128 (34108) 2008. [2] P. Koval, D. Foerster and O. Coulaud, J. Chem. Theory Comp. 6 (2654) 2010 . [3] D. Foerster, P. Koval, and D. Sánchez-Portal, J. Chem. Phys. 135, 74105 (2011) .

TT 61.11 Wed 13:15 MA 004

Modeling anisotropic organic molecules at patterned semiconductor surfaces — •Nicola Kleppmann and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Hybrid systems consisting of organic molecules at inorganic semiconductor surfaces are gaining increasing importance as thin film devices for optoelectronics. Their large charge carrier densities and tuneable resonance energies make them ideal candidates for semiconductor devices. However, the efficiency of such devices strongly depends on the self-organized structure formed by the adsorbed molecules, which depends, in turn, on the complex interplay of growth conditions and molecular properties. Recent ab initio calculations and experiments inspire us to examine the growth of sexiphenyl (6P) on ZnO(10-10) as a model system to understand self-organization of highly anisotropic molecules [1]. We develop a coarse-grained interaction hamiltonian of 6P molecules using a Gay-Berne potential and a linear quadrupole interaction term with additional substrate influence. We perform both equilibrium and non-equilibrium (growth) Monte Carlo simulations on a 2D lattice, where the rotational degrees of freedom of the molecules are continuous. We use these simulations to investigate orientational ordering in the condensed state, which is characterized by local descriptors such as order parameters and angular distributions.

[1] N. Kleppmann, and S. H. L. Klapp, submitted to JCP
[2] S. Bommel, N. Kleppmann et al., Nat Comm 5, 5388 (2014)

TT 62: Graphene: Dynamics (jointly with O, HL)

Time: Wednesday 10:30–13:00 Location: MA 041

TT 62.1 Wed 10:30 MA 041

Electron-phonon interactions and carrier transport in graphene — •tae yun kim[1], nicola marzari[2], and cheol-hwan park[1] — [1]Department of Physics, Seoul National University, Seoul 151-747, Korea — [2]Theory and Simulations of Materials (THEOS) and National Center for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The transport properties of graphene have received much attention partly for its possible applications in electronic devices. In particular, as recently reported, electron-phonon interactions are important in determining the intrinsic carrier transport properties [1,2]. Based on previous studies, we investigate further the carrier transport properties of graphene in terms of carrier density and other physical variables and find connection with experimental results on this matter.

This work was supported by Korean NRF funded by MSIP (Grant No. NRF-2013R1A1A1076141). Computational resources have been provided by Aspiring Researcher Program through Seoul National University (SNU) in 2014.

[1] C.-H. Park, N. Bonini, T. Sohier, G. Samsonidze, B. Kozinsky, M. Calandra, F. Mauri, and N. Marzari, Nano Lett. 14, 1113 (2014).
[2] T. Sohier, M. Calandra, C.-H. Park, N. Bonini, N. Marzari, and F. Mauri, Phys. Rev. B 90, 125414 (2014).

TT 62.2 Wed 10:45 MA 041

Non-linear luminescence and four-wave mixing from graphene, probed by femtosecond pulse shaping — •Richard Ciesielski[1], Alberto Comin[1], Matthias Handloser[1], Torben Winzer[2], Ermin Malic[2], and Achim Hartschuh[1] — [1]Ludwig-Maximilians-Universität, AK Hartschuh, Butenandtstr. 5-11, 81377 München — [2]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Ultrafast optical excitation of graphene leads to two main nonlinear emission signals in the visible. The first was described as incoherent non-linear photoluminescence (NLPL). The second results from near-degenerate four-wave mixing which is extraordinarily strong in graphene as compared to other materials. We investigated the two types of emission for different layer thickness using confocal microscopy and a 15 fs pulsed laser at 1.55 eV with a pulse shaper. Spectrally resolved autocorrelation scans revealed a continuously decreasing decay time of the NLPL from 1.2 eV towards 2.8 eV. Comparing the dynamics observed for different layers allows us to identify the influence of substrate induced doping. Finally, we were able to separate a weaker third contribution induced by the microscopic polarization of graphene

[1].

Financial support by the DFG through the Nanosystems Initiative Munich (NIM) and the ERC (NEWNANOSPEC) is gratefully acknowledged.

[1] T. Winzer, R. Ciesielski, M. Handloser et al., arXiv:1411.0531v1 (2014).

TT 62.3 Wed 11:00 MA 041

Microscopic description of intraband absorption in graphene — •Faris Kadi[1], Ermin Malic[1], Torben Winzer[1], Manfred Helm[2], Fabian Göttfert[2], Martin Mittendorff[2], Stephan Winnerl[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany — [2]Helmholtz- Zentrum Dresden-Rossendorf, Dresden, Germany

We present a microscopic explanation for the occurrence of the controversially discussed transient negative differential transmission observed in optical pump-probe measurements in graphene [1]. Within the density matrix formalism we investigate the transient transmission with respect to optical interband as well as phonon-assisted intraband transitions. While interband processes yield a positive contribution due to absorption bleaching, we find intraband transitions to decrease differential transmission. Interestingly, in the low excitation regime, the phonon-assisted absorption prevails over the absorption bleaching resulting in the experimentally observed negative differential transmission [2]. The zero-crossing occurs within the first hundreds of femtoseconds and is followed by a recovery of the transmission spectrum on a picosecond timescale in a good agreement with experimental observations. [1] S.Winnerl, F. Göttfert, M. Mittendorff, et al., Journal of Physics: Condensed Matter 25, 054202 (2013) [2] F. Kadi, T. Winzer, E. Malić, et al., Phys. Rev. Lett. 113, 035502, (2014)

TT 62.4 Wed 11:15 MA 041

Anisotropic Intravalley Scattering in Strongly Doped Graphene — •Daniela Dombrowski[1], Wouter Jolie[1], Sven Runte[1], Marin Petrović[2], Fabian Craes[1], Jürgen Klinkhammer[1], Marko Kralj[2], Predrag Lazić[3], Eran Sela[4], and Carsten Busse[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut za fiziku, Croatia — [3]Institut Ruđer Bošković, Croatia — [4]Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Israel

We perform Fourier-transform scanning tunneling spectroscopy (FT-STS) studies on Cs intercalated graphene on Ir(111). Angle-resolved photoemission spectroscopy (ARPES) measurements show, that the Cs strongly n-dopes graphene and shifts the Fermi level into the region of strong trigonal warping. We observe intervalley scattering and additionally a clear feature of intravalley scattering, which exhibits an anisotropic intensity distribution with dominant scattering in Γ-M direction.

In the linear region of the Dirac cone, conservation of pseudospin leads to the suppression of intravalley scattering since the direction of the pseudospin is either parallel or antiparallel to the momentum, thus the system has well defined chirality. This is no longer valid in the trigonal warping region near the Van-Hove singularity.

The FT-STS results are supplemented by density functional calculations of the electronic band structure and simulations of the scattering pattern based on the T-matrix theory.

TT 62.5 Wed 11:30 MA 041

Theory of coherent light emission in graphene — •Roland Jago, Torben Winzer, Andreas Knorr, and Ermin Malic — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Within the density matrix formalism we present a microscopic and full quantized theoretical description of the coupled carrier, phonon and photon dynamics in graphene implemented in a photonic crystal nanocavity. We demonstrate that under strong optical excitation a spectrally broad and long-lived population inversion can be achieved. In the case of free-standing graphene non-radiative Coulomb-induced carrier-recombination on a femtosecond time scale prevents an efficient emission of coherent photons. To partially suppress this ultrafast recombination, we propose to support graphene on a substrate having high-dielectric screening. In this case, our calculations reveal a temporarily extended population inversion, that remains stable up to some tens of picoseconds under realistic conditions. In particular we observe the emission of coherent laser light suggesting graphene as gain medium for lasers [2].

[1] T. Winzer, E. Malic and A. Knorr, Phys. Rev. B 87, 165413 (2013) [2] R. Jago, T. Winzer, A. Knorr and E. Malic, arXiv:1409.8182 (2014)

TT 62.6 Wed 11:45 MA 041

Phonon dynamics of graphene on copper substrate — •Naira S. Grigoryan, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretical Physics, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

In the framework of density functional theoretical calculations, the lattice dynamical properties of graphene with and without a Cu(111) substrate have been investigated and analyzed using our in-house code for highly excited valence electron systems (CHIVES). We find that the lattice dynamics exhibits large sensitivity to the presence of copper. In particular, the appearance of a nearly dispersionless phonon branch at ~1.5THz makes this system a potential mirror for light molecules. We further show that there is a lifting of the degeneracy of the ZO and ZA modes at the M- point.

TT 62.7 Wed 12:00 MA 041

Non-equilibrium Carrier Relaxation in Graphene investigated with tr-ARPES — •Mariana Chavez Cervantes[1], Raghu Tomar[1], Hubertus Bromberger[1], Haiyun Liu[1], Stefan Link[2], Ulrich Starke[2], Andrea Cavalleri[1,3], and Isabella Gierz[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, United Kingdom

We used time- and angle-resolved photoemission spectroscopy (tr-ARPES) based on high order harmonics generation for the extreme ultra-violet (XUV) probe to investigate the relaxation of photo-excited carriers in quasi-freestanding epitaxial graphene samples. From the data we determined the energy dependence of the scattering rate that, according to Ref. [1,2], is predicted to follow the imaginary part of the *equilibrium* self-energy. In order to test this hypothesis we compare the scattering rate measured at different sample temperatures and for different pump fluences with the equilibrium self-energy determined from high-resolution static ARPES experiments as described in Ref. [3,4].

[1] M. Sentef et al., Phys. Rev. X 3, 041033 (2013)
[2] A. F. Kemper et al., Phys. Rev. B 90, 075126 (2014)
[3] A. Bostwick et al., Nat. Phys. 3, 36 (2007)
[4] I. Gierz et al., Faraday Disc. 171 (1), 311 (2014)

Invited Talk TT 62.8 Wed 12:15 MA 041

Electronic structure and electron dynamics in two-dimensional materials — •Philip Hofmann — Department of Physics and Astronomy, Aarhus University

Two-dimensional materials can be grown epitaxially and in high quality on different substrates, and this can be exploited to study their electronic structure and different many-body effects. In this talk I will review the growth and electronic properties of epitaxial graphene, bilayer graphene and single-layer MoS_2. Specifically, I will focus on the electronic structure of these materials as studied by angle-resolved photoemission spectroscopy. This technique does not only give access to the materials' band structure but also to many-body effects such as the electron-electron and electron-phonon interaction. This is particularly so for the time-resolved variety of the technique in which the carrier dynamics can be followed in real time.

TT 62.9 Wed 12:45 MA 041

Dirac carrier thermalization on the sub 10fs timescale observed by tr-ARPES — •Sven Aeschlimann[1,2], Mariana Chavez Cervantes[1], Francesca Calegari[1,3], Cephise Cacho[4], Emma Springate[4], Stefan Link[2], Ulrich Starke[2], Klaus Kern[2,5], Andrea Cavalleri[1,6], Christian R. Ast[2], and Isabella Gierz[1] — [1]MPI for the Structure and Dynamics of Matter, Hamburg, Germany — [2]MPI for Solid State Research, Stuttgart, Germany — [3]IFN, Consiglio Nazionale delle Ricerche, Milano, Italy — [4]Central Laser Facility, STFC Rutherford Appleton Laboratory, Harwell, United Kingdom — [5]EPFL, Lausanne, Switzerland — [6]University of Oxford, United Kingdom

We used time- and angle-resolved photoemission spectroscopy (tr-ARPES) with extreme ultra-violet (XUV) probe pulses from high order harmonics generation (HHG) to observe the ultrafast electron dynamics in photo-excited quasi-freestanding epitaxial graphene monolayers.

By the use of the hollow core fiber compression technique, we produced 8 fs pulses, which are utilized both for driving HHG and for photo-excitation. These ultrashort pulses allowed us to observe the initial thermalization of photo-excited carriers via electron-electron scattering with unprecedented temporal resolution. We find that, at early times, the carrier distribution neither follows a Fermi-Dirac distribution nor the non-equilibrium distribution expected for a population-inverted state [1]. We attribute this to the short duration of the pump pulse on the order of the electron-electron scattering time.

[1] I. Gierz et al., Nature Materials 12, 1119 (2013)

TT 63: Topological Insulators: Theory (jointly with HL, DS, MA, O)

Time: Wednesday 9:30–11:30 Location: ER 270

TT 63.1 Wed 9:30 ER 270

Weyl and Dirac semimetals: A platform for new interface phenomena — •Adolfo G. Grushin[1], Jorn W. F. Venderbos[2], and Jens H. Bardarson[3] — [1]Max Planck Institute for the physics of Complex Systems, Dresden, Germany — [2]Massachusetts Institute of Technology, Cambridge, MA, USA — [3]Max Planck Institute for the physics of Complex Systems, Dresden, Germany

The Weyl semimetal (WSM) state is sometimes loosely referred to as the three-dimensional cousin of graphene since its low energy theory is described by an even number of copies of the Weyl Hamiltonian. Closely related to WSM, the Dirac semimetals hosts the Weyl nodes at the same point in the Brillouin Zone and it is realised in Cd_3As_2 and Na_3Bi compounds. In this talk I will explore the rich surface state physics that these states can host and how can it be probed, including coexistence of Dirac and Fermi arc states at the topological insulator-weyl semimetal interfaces as well as signatures of the chiral anomaly.

TT 63.2 Wed 9:45 ER 270

Spin chirality tuning and Weyl semimetal in strained $HgS_{1-x}Te_x$ — •Tomáš Rauch[1], Steven Achilles[1], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle (Saale), Germany

We have theoretically investigated the phase diagram of $HgS_{1-x}Te_x$. The parameters which have been varied are the concentration x and the in-plane strain, which could be applied by an appropriate substrate in an experiment. In the topological phase diagram we found a normal metallic phase, two topological insulator phases with different spin chiralities of the surface states and a Weyl semi-metal phase. The phases have been probed by calculating topological invariants and the dispersion of the surface states for both crystal terminations of the (001) surface by an *ab-initio* based tight-binding model.

TT 63.3 Wed 10:00 ER 270

Topological phases in (interfacial) phase-change materials — •Peter Schmitz, Wei Zhang, and Riccardo Mazzarello — Institute for Theoretical Solid State Physics, RWTH Aachen University

We investigate the topological, spectral and structural properties of $[Sb_2Te_3]_x[GeTe]_y$ (GST) compounds, some of which are interfacial phase change materials (IPCMs), as a function of strain and stacking sequence by performing a DFT study of bulk and slab models and discuss the relevance of a 3D (topological) Dirac semimetal phase ((T)DSM), eg. to GST225.

IPCMs can perform fast reversible transitions, induced by electric fields or heat, between crystalline states of different stacking. Since they also possess strong spin-orbit coupling and a strong topological insulator (STI) + normal insulator(NI) layering, they are a promising platform to investigate nontrivial interface states and direct applications to data storage in terms of switching topological phases. Until now they were shown to exhibit STIs and *unstable* DSM-like critical states corresponding to STI/NI transitions [1]. Then recently [2] a *robust* TDSM phase was predicted for crystals having certain rotational symmetries: The STI/NI transition point can be extended to a line and 2 Dirac points appear in the bulk spectrum.

Analyzing whether such phases can be obtained in GST compounds is also interesting since the problem of a TDSM in a multilayer structure has not yet been discussed.

[1] J. Tominaga et al, Adv. Mat. Inter. 1 (2014);
[2] B. Yang and N. Nagaosa, Nature Commun. 5, 4898 (2014)

TT 63.4 Wed 10:15 ER 270

Effect of Bi bilayers on the topological states of Bi_2Se_3: A first-principles study — Kirsten Govaerts[1], Kyungwha Park[2], Christophe De Beule[1], Dirk Lamoen[1], and •Bart Partoens[1] — [1]CMT-group and EMAT, University of Antwerp, Belgium — [2]Virginia Tech, Department of Physics, USA

Bi_2Se_3 and vice versa, has not been explored much. Bi bilayers are often present between the quintuple layers of Bi_2Se_3, since $(Bi_2)_n(Bi_2Se_3)_m$ form stable ground-state structures. Moreover, Bi_2Se_3 is a good substrate for growing ultrathin Bi bilayers. By first-principles techniques, we first show that there is no preferable surface termination by either Bi or Se. Next, we investigate the electronic structure of Bi bilayers on top of, or inside a Bi_2Se_3 slab. If the Bi bilayers are on top, we observe a charge transfer to the quintuple layers that increases the binding energy of the surface Dirac cones. The extra states, originating from the Bi bilayers, were declared to form a topological Dirac cone, but here we show that these are ordinary Rashba-split states. This result, together with the appearance of a new Dirac cone that is localized slightly deeper, might necessitate the reinterpretation of several experimental results. When the Bi bilayers are located inside the Bi_2Se_3 slab, they tend to split the slab into two topological insulators with clear surface states. Interface states can also be observed, but an energy gap persists because of strong coupling between the neighboring quintuple layers and the Bi bilayers.

TT 63.5 Wed 10:30 ER 270

Topological states in α-Sn and HgTe quantum wells: a comparison of ab-initio results — •Sebastian Küfner and Friedhelm Bechstedt — Friedrich Schiller Universität Jena

Quantum well (QW) structures based on HgTe are theroretically predicted and experimentally verified to exhibit the quantum-spin Hall phase. Despite the similarities of the bulk band structures, studies of α-Sn QW structures are missing. We compare the properties of QW structures made by the different zero-gap semiconductors α-Sn and HgTe, but both sandwiched in nearly lattice-matched CdTe barriers by means of first-principles calculations including quasiparticle corrections and spin-orbit interaction. The two well materials possess different space groups O_h^7 (diamond structure) and T_d^2 (zinc-blende structure). The spin-orbit interaction, in particular that in the p-derived valence states, is different due to the contribution of both atoms in the unit cell (α-Sn) and mainly the anion (HgTe) to the states at the top of the valence bands, and the different local electrostatic properties due to the different bonding character in the QW layers and their interfaces with the CdTe barrier material. We investigate the similarities and differences of the two embedded zero-gap semiconductors on the formation of quantum-well, edge and interface states in detail.

TT 63.6 Wed 10:45 ER 270

Quasiparticle band structure of the topological insulator Bi_2Se_3 — •Tobias Förster, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Bi_2Se_3 is a prototype topological insulator. Its simple surface band structure with only one Dirac point makes it an ideal system for exploring the properties of topological surface states. Up to now, the vast majority of theoretical investigations of the electronic structure of Bi_2Se_3 has utilized DFT calculations. In Bi_2Se_3 and related compounds, however, many body perturbation theory in the GW approximation yields both quantitative and qualitative quasiparticle corrections of the DFT bulk band structures [1].

Here we discuss results for bulk Bi_2Se_3 from GW calculations employing a localized basis as well as from a perturbative LDA+GdW approach [2]. The latter provides a numerically very efficient method for the calculation of quasiparticle corrections with only slightly reduced precision compared to GW. The applicability of the LDA+GdW formalism to the Bi_2Se_3 surface with the Dirac state will also be ad-

dressed.

[1] I. Aguilera *et al.*, Phys. Rev. B **88**, 045206 (2013)
[2] M. Rohlfing, Phys. Rev. B **82**, 205127 (2010)

TT 63.7 Wed 11:00 ER 270

Calculation of topological invariants from a maximally localized Wannier functions derived model Hamiltonian — •Patrick M. Buhl, Chengwang Niu, Yuriy Mokrousov, Daniel Wortmann, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Using density-functional methods it is possible to provide an accurate description of topological phases in complex materials. We demonstrate how topological characterization can be performed in a unified manner based on Wannier functions generated from the full-potential linearized augmented plane-wave method as implemented in the FLEUR code [1]. Taking as examples bcc Fe, Na_3Bi and PbTe we compute various topological invariants and identify topologically non-trivial points in the electronic structure of these materials in bulk and their close relation to the surface electronic structure. In particular, we focus on the Weyl semimetallic phase as a transitional phase between various topological phases in the same material and on the role of the Weyl points in the electronic structure for topological properties. Financial support by the HGF-YIG Programme VH-NG-513 and SPP 1666 of the DFG is gratefully acknowledged.

[1] F. Freimuth *et al.*, Phys. Rev. B **78**, 035120 (2008)

TT 63.8 Wed 11:15 ER 270

Functionalized Bismuth Films: Giant Gap Quantum Spin Hall and Valley-Polarized Quantum Anomalous Hall States — •Chengwang Niu, Gustav Bihlmayer, Hongbin Zhang, Daniel Wortmann, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The search for new large band gap quantum spin Hall (QSH) and quantum anomalous Hall (QAH) insulators is critical for their realistic applications at room temperature [1,2]. Here we predict, based on first principles calculations, that the band gap of QSH and QAH states can be as large as 1.01 eV and 0.35 eV in an H-decorated Bi(111) film [3]. The origin of this giant band gap lies both in the large spin-orbit interaction of Bi and the H-mediated exceptional electronic and structural properties. Moreover, we find that the QAH state also possesses the properties of quantum valley Hall state, thus intrinsically realising the so-called valley-polarized QAH effect. We further investigate the realization of large gap QSH and QAH states in an H-decorated Bi($\bar{1}$10) film and X-decorated (X=F, Cl, Br, and I) Bi(111) films.

This work was supported by the Priority Program 1666 of the DFG and project VH-NG-513 of the HGF.

[1]M. Hasan and C. Kane, Rev. Mod. Phys. **82**, 3045 (2010).
[2]X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).
[3]Chengwang Niu, Gustav Bihlmayer, Hongbin Zhang, Daniel Wortmann, Stefan Blügel, and Yuriy Mokrousov, submitted.

TT 64: Quantum Information Systems: Mostly Concepts (jointly with HL)

Time: Wednesday 11:00–13:00 Location: EW 202

TT 64.1 Wed 11:00 EW 202

Cold atom - semiconductor hybrid quantum system — •Jan-Philipp Jahn[1], Mathieu Munsch[1], Lucas Beguin[1], Andreas Kuhlmann[1], Aline Faber[1], Tobias Kampschulte[1], Andreas Jöckel[1], Armando Rastelli[2], Fei Ding[3], Oliver G. Schmidt[3], Nicolas Sangouard[1], Philipp Treutlein[1], and Richard J. Warburton[1] — [1]University of Basel, Switzerland — [2]Johannes-Kepler University Linz, Austria — [3]IFW Dresden, Germany

Semiconductor quantum dots are excellent single-photon sources, providing triggered single-photon emission at a high rate and with high spectral purity [1]. Independently, atomic ensembles have emerged as one of the best quantum memories for single photons, providing high efficiency storage and long memory lifetimes [2]. In this project, we combine these two physical systems to exploit the best features from both worlds. On the one hand, we have characterized a new type of self-assembled GaAs/AlGaAs quantum dots that emit narrowband ($\Delta\nu$ = 500 MHz) single-photons at a wavelength compatible with Rb atoms. Fine tuning of the photon frequency is achieved via strain. This allows us to perform spectroscopy of the Rb D2-line at the single-photon level, proving that we can address the different hyperfine transitions. On the other hand, we have developed a detailed theory of an EIT-based memory scheme in a dense ultracold ensemble of 87Rb atoms (OD>150) that achieves storage-and-retrieval efficiency exceeding 28% [3].

[1] R. J. Warburton, Nature Mater. 121, 483-493 (2013) [2] F. Bussières et al., J. Mod. Opt. 60, 1519 (2013) [3] M. T. Rakher et al., Phys. Rev. A 88, 053834 (2013)

TT 64.2 Wed 11:15 EW 202

Surface Acoustic Waves as a versatile tool for quantum information processing with solid-state spin qubits — •Martin J. A. Schuetz[1], Eric M. Kessler[2,3], J. Ignacio Cirac[1], Mikhail D. Lukin[2,3], Lieven M. K. Vandersypen[4], and Géza Giedke[1,5] — [1]Max-Planck-Institut für Quantenoptik, H.-Kopfermann-Str 1, D-85748 Garching — [2]ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138, USA — [3]Physics Department, Harvard University, Cambridge, Massachusetts 02318, USA — [4]Kavli Institute of NanoScience, TU Delft, P.O. Box 5046, 2600 GA Delft, The Netherlands — [5]Donostia International Physics Center, Paseo Manuel de Lardizabal 4, E-20018 San Sebastian

Surface acoustic waves (SAW) offer a great variety of applications in the context of solid-state quantum information processing (QIP). The use of SAWs as transport shuttles for single electrons has been demonstrated, high-quality cavities for SAW can be fabricated, and their quantum nature has been explored coupling them to superconducting qubits.

We investigate theoretically the use of SAWs for QIP with spin qubits in GaAs quantum dots. We show that strong coupling between the qubit and SAW cavities is feasible with current cavity designs. We investigate the viability of "quantum acoustics" in this setting, where phononic cavities are used to couple spin qubits and phonons serve as propagating carriers of quantum information. Possibilities to extend these results to other spin qubits such as NV centers in diamond are discussed.

TT 64.3 Wed 11:30 EW 202

Creating and controlling entanglement using coherent time-delayed feedback — •Sven Moritz Hein, Franz Schulze, Alexander Carmele, and Andreas Knorr — Technische Universität Berlin, Institut für theoretische Physik, Nichtlineare Optik und Quantenelektronik, Hardenbergstraße 36, 10623 Berlin, Germany

Entanglement is a quantum-mechanical property interesting from a fundamental point of view as well as for future applications in quantum information science. We propose to use time-delayed quantum-coherent feedback to create and control entanglement between quantum-mechanical objects.

In classical physics, feedback schemes with a distinct feedback delay[1] are successfully applied to control unstable states and periodic orbits. We demonstrate by numerical simulations that this concept can be transferred to the quantum regime. Here, it can be used to enhance the entanglement of photons from a biexciton cascade[2] and also entangle cavities and other quantum nodes in a quantum network. To preserve quantum coherence, the feedback will be modeled in a fully quantum-mechanical way without the use of measurements.

[1] K. Pyragas, Phys. Lett. A 170, 421–428 (1992)
[2] S. M. Hein, et al., Phys. Rev. Lett. 113, 027401 (2014)

TT 64.4 Wed 11:45 EW 202

Temporal shaping of Gaussian single photon pulses — •Emanuel Peinke[1], Gaston Hornecker[2], Julien Claudon[1], Alexia Auffèves[2], and Jean-Michel Gérard[1] — [1]CEA/CNRS joint team "Nanophysics and Semiconductors", INAC, CEA and Université Grenoble Alpes, Grenoble, France — [2]CEA/CNRS joint team "Nanophysics and Semiconductors", Institut Néel, CNRS and Université Grenoble Alpes, Grenoble, France

Single photon pulses with a Gaussian temporal envelope constitute an important resource for optical quantum information processing [1].

We propose here a scheme to shape single photon pulses with high fidelity using a two-level emitter (e.g. a quantum dot (QD)) coupled to a frequency-tunable microcavity. By controlling the cavity resonance frequency on a time-scale shorter than the typical emitter spontaneous emission time, one controls the instantaneous emission rate and thus the temporal envelope of the emitted photon. For realistic experimental parameters, we show that nearly ideal Gaussian pulses can be generated with QD-semiconductor systems and superconducting Josephson circuits.

[1] P. P. Rohde, T. C. Ralph, and M. A. Nielsen. Optimal photons for quantum- information processing. Phys. Rev. A, 72:052332, Nov 2005.

TT 64.5 Wed 12:00 EW 202

Electric dipole spin resonance in the presence of valley degeneracy — •Marko Rancic and Guido Burkard — University of Konstanz

We theoretically investigate the electric dipole spin resonance (EDSR) in a single Si/SiGe quantum dot in the presence of a magnetic field gradient, e.g., produced by a micomagnet. The control of electron spin states can be achieved by applying an oscillatory electric field, which induces periodic back and forth motion of the electron spin inside the quantum dot. This motion inside a magnetic field gradient, produces an effective periodic in-plane magnetic field, and allows for driven spin rotations near resonance. By solving a Lindblad master equation, we discuss possible electron spin relaxation and decoherence mechanisms relevant to EDSR. In Si there is 5% of naturally occurring nuclear spin 1/2 isotope, which causes the electron spin to decohere. Nuclear spins are included in our model through the additional random Overhauser magnetic field. Furthermore, a valley dependent g-factor, combined with intervalley scattering gives rise to another electron spin decoherence mechanism. The goal of our study is to describe the efficiency of a spin echo sequence in the presence of all mentioned relaxation and decoherence mechanisms.

TT 64.6 Wed 12:15 EW 202

Resonant exchange qubit under influence of electrical noise — •Maximilian Russ and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

In this work we investigate the influence of electrical charge noise on a resonant exchange (RX) qubit in a triple quantum dot. This RX qubit is a variation of the exchange-only qubit [1] which responds only to a narrow-band resonant frequency [2,3]. Our noise model includes uncorrelated charge noise in each quantum dot giving rise to two independent (noisy) bias parameters. We calculate the energy splitting of the two qubit states as a function of these two bias detuning parameters to find "sweet spots", where the noise suppression is maximized. Our investigation shows that such sweet spots exist within the low bias regime, in which the bias detuning parameters have the same magnitude as the hopping parameters. The location of the sweet spots depends on the bias detuning and the hopping asymmetry between the quantum dots.

[1] D. P. DiVincenzo et al., Nature **408**, 339 (2000).
[2] J. Medford et al., Phys. Rev. Lett. **111**, 050501 (2013).
[3] J. M. Taylor, V. Srinivasa, and J. Medford, Phys. Rev. Lett. **111**, 050502 (2013).

TT 64.7 Wed 12:30 EW 202

Electrically controlled echo sequences for the exchange-only qubit — •Niklas Rohling and Guido Burkard — Department of Physics, University of Konstanz, Germany

We consider a model of an exchange-only qubit [1] in a triple quantum dot under the influence of the surrounding nuclear spin bath, which we describe by an inhomogeneous Overhauser field. This field can lead to decoherence and leakage out of the logical qubit space. When a strong external magnetic field is applied, the spin in each of the quantum dots precess effectively about the same axis. In this case, only one leakage state has to be taken into account [2]. For this situation, we present a purely exchange-based pulse sequence that corrects decoherence as well as leakage as long as the Overhauser field varies slowly compared to the pulse times. As the pulses rely on the exchange interaction, they can be electrically tuned similarly to the quantum gates of the qubit [1]. For the case of a well-known initial state, we further refine the sequence to allow for first-order correction of errors in the applied pulses in analogy to the Carr-Purcell-Meiboom-Gill sequence known from spin resonance techniques.

[1] D. P. DiVincenzo, D. Bacon, J. Kempe, G. Burkard, and K. B. Whaley, Nature **408**, 339 (2000)
[2] J.-T. Hung, J. Fei, M. Friesen, and X. Hu, Phys. Rev. B **90**, 045308 (2014)

TT 64.8 Wed 12:45 EW 202

Influence of Hyperfine Interaction on the Entanglement of Photons Generated by Biexciton Recombination — •Erik Welander, Julia Hildmann, and Guido Burkard — Department of Physics, University of Konstanz, Germany

The quantum state of the emitted light from the cascade recombination of a biexciton in a quantum dot is theoretically investigated including exciton fine structure splitting (FSS) and electron-nuclear spin hyperfine interactions. In an ideal situation, the emitted photons are entangled in polarization making the biexciton recombination process a candidate source of entangled photons necessary for the growing field of quantum communication and computation. The coherence of the exciton states in real quantum dots is affected by a finite FSS and the hyperfine interactions via the effective magnetic field known as the Overhauser field. We investigate the influence of both sources of decoherence and find that the FSS combined with a stochastic exciton lifetime is responsible for the main loss of entanglement. Furthermore, we examine the possibility of reducing the decoherence from the Overhauser field by partially polarizing the nuclear spins and applying an external magnetic field. We find that an increase in entanglement depends on the degree as well as the direction of nuclear spin polarization.

TT 65: Low-Dimensional Systems: 1D – Theory

Time: Wednesday 15:00–19:15 Location: H 0104

Topical Talk TT 65.1 Wed 15:00 H 0104

Strong Correlations in Disordered One-Dimensional Systems — •Christoph Karrasch and Joel Moore — UC Berkeley, USA

We investigate the effects of strong electronic correlations in disordered one-dimensional systems such as XXZ spin chains. In order to study the problem from different perspectives, both semi-analytical methods (the functional renormalization group) and purely computational techniques (the density matrix renormalization group) are employed. First, we briefly discuss a recently-introduced 'disentangler' which allows to carry out finite-temperature dynamical DMRG simulations up to larger times. Thereafter, we study a variety of questions: How is Luttinger liquid behavior cut off by weak disorder? Are there new power laws? Can we identify many-body localized and metallic phases if the disorder is strong, and can we learn something about the transition between the two?

TT 65.2 Wed 15:30 H 0104

Efficient time-evolution for long-ranged one-dimensional Hamiltonians — •Frank Pollmann[1], Mike Zaletel[2], Roger S. K. Mong[3], Christoph Karrasch[2], and Joel E. Moore[2] — [1]Max-Planck-Institut f'ur Physik komplexer Systeme, 01187 Dresden, Germany — [2]University of California, Berkeley, California 94720, USA — [3]California Institute of Technology, Pasadena, California 91125, USA

We introduce a numerical algorithm to simulate the time evolution of a matrix product state under a long-ranged Hamiltonian. In the effectively one-dimensional representation of a system by matrix product states, long-ranged interactions are necessary to simulate not just many physical interactions but also higher- dimensional problems with short-ranged interactions. Since our method overcomes the restriction to short- ranged Hamiltonians of most existing methods, it proves particularly useful for studying the dynamics of both power-law interacting one-dimensional systems, such as Coulombic and dipolar systems, and quasi two- dimensional systems, such as strips or cylinders. First, we benchmark the method by verifying a long-standing theoretical prediction for the dynamical correlation functions of the Haldane-Shastry model. Second, we simulate the time evolution of an expanding cloud

of particles in the two-dimensional Bose-Hubbard model, a subject of several recent experiments.

TT 65.3 Wed 15:45 H 0104

Rashba coupling and magnetic order in correlated helical liquids — •Martin Hohenadler and Fakher Assaad — Universität Würzburg, Germany

We study strongly correlated helical liquids with and without Rashba coupling using quantum Monte Carlo simulations of the Kane-Mele model with a Hubbard interaction at the edge. Independent of the Rashba coupling, we find that interactions enhance spin correlations and suppress the spectral weight at the Fermi level. For sufficiently strong interactions, a gap can be observed in the single-particle spectral function. However, based on a finite-size scaling analysis and theoretical arguments, we argue that this gap is closed by order parameter fluctuations in the Luttinger liquid phase even at zero temperature, and filled in by thermally induced kinks in the order parameter in the Mott phase at finite temperatures. While the bosonization suggests an umklapp-driven Mott transition only in the presence of Rashba coupling and hence an important impact of the latter, our numerical results are almost unaffected by Rashba coupling even at low temperatures.

TT 65.4 Wed 16:00 H 0104

Effective ladder models for correlated wires on substrates — •Anas Abdelwahab[1], Eric Jeckelmann[1], and Martin Hohenadler[2] — [1]Leibniz Universität Hannover, Germany — [2]Universität Würzburg, Germany

The study of correlated quantum wires deposited on a substrate constitutes a challenge for existing analytical and numerical methods. We show that these systems can be mapped onto effective n-leg ladder models, which can then be investigated thoroughly using well-established methods for quasi-one-dimensional systems, such as the density-matrix renormalization group (DMRG) or bosonization. The possibilities and limitations of this approach are demonstrated with exact results for non-interacting systems as well as with DMRG and quantum Monte Carlo calculations for interacting wires. We present results for a two-leg effective model [1] and discuss the modeling of Luttinger liquids on semiconducting substrates. Support from the DFG through the Research Unit FOR 1807 is gratefully acknowledged.

[1] A. Abdelwahab, E. Jeckelmann, and M. Hohenadler, arXiv:1409.7315

TT 65.5 Wed 16:15 H 0104

Spin-charge-separated quasi-particles in 1D quantum fluids — •Imke Schneider[1], Rodrigo G. Pereira[2], and Fabian H. Essler[3] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Instituto de Fisica de Sao Carlos, Universidade de Sao Paulo, C.P. 369, Sao Carlos, SP, 13560-970, Brazil — [3]The Rudolf Peierls Centre for Theoretical Physics, Oxford University, Oxford OX1 3NP, United Kingdom

Interacting one-dimensional quantum fluids are well-studied examples of systems in which the Fermi liquid paradigm of electron-like quasi-particles is known to break down. Instead, Luttinger liquid theory predicts separate spin- and charge-density waves - bosonic in nature - as the fundamental collective excitations at low energies.

Recently, the idea of fermionic quasi-particles for 1D quantum fluids was revived by the interest in dynamics beyond the Luttinger liquid paradigm. Here we propose a constructive approach to introduce fermionic quasi-particles for two-component Luttinger liquids. We point out that a model with weakly interacting fermionic quasi-particles at low energies - a good starting point for the universal theory of nonlinear Luttinger liquids - is a double Luther-Emery Point which can only be reached by fine tuning of strong interactions. Using density matrix renormalization group(DMRG) methods, we search for a lattice realization of this point in an extended Hubbard model with longer-range density-density and spin exchange interactions.

TT 65.6 Wed 16:30 H 0104

Exact calculation of thermal correlation functions of the antiferromagnetic Heisenberg chain at large distances — •Frank Göhmann and Maxime Dugave — Bergische Universität Wuppertal

Thermal correlation functions of integrable models in the thermodynamic limit can be expanded in a basis of eigenstates of the corresponding quantum transfer matrix. This provides an asymptotic expansion in which every term is determined by a correlation length and by an amplitude. We have derived exact formulae for the amplitudes for the longitudinal and transverse correlation functions of the anisotropic Heisenberg chain in the spin liquid regime as functions of temperature and magnetic field. In the zero temperature limit infinitely many correlation lengths diverge, while the amplitudes decay algebraically with temperature, with the same critical exponents that determine the spatial decay of the ground state correlation functions. We have summed up these infinitely many terms exactly and, as a result, have obtained efficient expressions for the amplitudes of the critical correlation functions, generalizing well-known formulae of Lukyanov to finite magnetic fields.

TT 65.7 Wed 16:45 H 0104

Form Factor Expansions for the XXZ Chain in the Massive Regime — •Maxime Dugave and Frank Göhmann — Bergische Universität Wuppertal

We discuss the form factor approach to correlation functions of the integrable anisotropic spin-1/2 Heisenberg chain in the massive regime at zero temperature.

Using the transfer-matrix technique and Bethe ansatz, we characterize the spectrum of the Hamiltonian in the thermodynamic limit. By analyzing the non-linear integral equations which describe excited states, we rederive the classification of excitations found by Babelon, De Vega and Viallet (1983) and correct an error in the higher-level Bethe equations obtained in this classical work.

This lays the basis for the calculation of exact expressions for matrix elements of local operators in the thermodynamic limit. In the 2-particle case, we find agreement with results from the vertex operator approach (Jimbo and Miwa (1995), Lashkevich (2002)). We eventually obtain the leading large-distance asymptotics of the longitudinal correlation functions by a saddle-point integration.

15 min. break.

TT 65.8 Wed 17:15 H 0104

Dynamics of S=1 Heisenberg chains at finite temperatures — •Thomas Köhler[1], Salvatore R. Manmana[1], Stephan C. Kramer[2], Andreas Honecker[3], and Thomas Pruschke[1] — [1]Institut f. Theoretische Physik, Universität Göttingen — [2]Max-Planck-Institut f. biophysikalische Chemie, Göttingen — [3]LPTM, Université de Cergy-Pontoise, France

We compute dynamical spectral functions for S=1 Heisenberg systems at finite temperatures T using matrix product state (MPS) approaches. This is achieved by parallelizing the time evolution on GPUs, and via a linear prediction ansatz on the time evolution results. We discuss the effect of temperature on the spectral functions and provide an outlook on the fate of the Haldane state upon increasing T.

TT 65.9 Wed 17:30 H 0104

Spectral functions of one-dimensional quantum magnets — •Alexander C. Tiegel[1], Salvatore R. Manmana[1], Thomas Pruschke[1], and Andreas Honecker[2] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]LPTM, Université de Cergy-Pontoise, France

We present numerical results for experimentally relevant spectral functions of one-dimensional strongly correlated quantum systems. We focus on the electron spin resonance (ESR) modes of spin-1/2 XXZ Heisenberg chains with Dzyaloshinskii-Moriya interactions in magnetic fields at both zero and finite temperature. The spectral functions are computed directly in the frequency domain via a Chebyshev expansion of the Green's function in a density-matrix renormalization group (DMRG) framework using matrix product states (MPS). At finite temperature, the method is based on a purification of the density operator by exploiting a Liouville space formulation of the dynamics. Our results are compared to field-theoretical descriptions from the literature.

TT 65.10 Wed 17:45 H 0104

Work distribution in quantum quenches of the anistoropic Heisenberg (XXZ) chain — •Paolo Pietro Mazza[1], Elena Canovi[2], Vincenzo Alba[3], and Masudul Haque[4] — [1]Max Planck Institute for Physics of Complex Systems, Dresden — [2]Max Planck Research Department for Structural Dynamics, University of Hamburg-CFEL, Hamburg — [3]Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität Munich — [4]Max Planck Institute for Physics of Complex Systems, Dresden

An important feature of a quantum quench is the distribution of overlaps of the initial state with the eigenstates of the final Hamiltonian. This distribution of overlaps is closely related to the distribution of work done in a quantum quench. We will present a study of the overlap distribution in the XXZ spin chain. We will consider quenches of the anisotropy parameter and describe which eigenstates get excited in such quenches.

TT 65.11 Wed 18:00 H 0104

Minimally entangled typical thermal states and matrix product purifications for the simulation of strongly-correlated quantum systems at T>0 — Moritz Binder[1] and •Thomas Barthel[2] — [1]LMU München — [2]LPTMS, Université Paris-Sud and CNRS

We describe different approaches for the study of equilibrium states and finite-temperature response functions of strongly-correlated quantum many-body systems in the framework of the density matrix renormalization group (DMRG). One is based on matrix product purifications. An alternative are so-called minimally entangled typical thermal states (METTS) which combine DMRG with sampling. We compare and explain the efficiencies of these methods and new variants using the spin-1/2 XXZ chain and the 1D Bose-Hubbard model as examples.

TT 65.12 Wed 18:15 H 0104

Exchange couplings in spin chains — •Kira Riedl, Harald O. Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

Within the framework of density functional theory, we investigate the variation of exchange couplings in $SrCuO_2$ and Sr_2CuO_3 spin chains[1] upon doping[2] with magnetic and non-magnetic impurities. In this talk we shall discuss the various cases and compare with experimental results.

This work is being performed in collaboration with C. Rüegg.

[1] N. Hlubek, X. Zotos, S. Singh, R. Saint-Martin, A. Revcolevschi, B. Büchner, and C. Hess, J. Stat. Mech. **12**, P03006 (2012).
[2] K. Karmakar, A. Singh, S. Singh, A. Pool, and C. Rüegg, Cryst. Growth Des. **14**, 1184 (2014).

TT 65.13 Wed 18:30 H 0104

Scaling of critical wave functions at topological Anderson transitions in 1D — •Eoin Quinn[1], Thomas Cope[2], Jens H. Bardarson[1], and Alexander Ossipov[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]University of Nottingham, Nottingham, United Kingdom

Topological Anderson transitions occur when a change in the strength of a system's disorder takes the system between two topologically distinct phases. The critical wavefunctions at such transitions display universal features. We present analytical and numerical results on the boundary scaling of critical wavefunctions for systems that are quasi-1D.

TT 65.14 Wed 18:45 H 0104

Quench dynamics of the entanglement spectrum in a dimerized chain — •Yi-Hao Jhu[1,4], Pochung Chen[1,2], Ming-Chiang Chung[2,3], and Frank Pollmann[4] — [1]Physics Department, National Tsing Hua University, Hsinchu, 30013, Taiwan — [2]Physics Division, National Center for Theoretical Science, Hsinchu, 30013, Taiwan — [3]Department of Physics, National Chung Hsing University, Taichung, 40227, Taiwan — [4]Max-Planck-Institut für Physik komplexer Systeme, Dresden, 01187, Germany

We investigate the quench dynamics of a dimerized chain of spin less fermions in the presence of nearest-neighbor interactions. We first obtain the ground state phase diagram and focus on the stability of a topological phase of "Su-Schrieffer-Heeger" type. We then study the evolution of the entanglement spectrum following a global quench in which the dimerization strength is changed. In the non-interacting case, degeneracies in the spectrum revive at long times which indicates the stability of the topological properties. When interactions between the fermions are present, the state thermalizes and the degeneracies are lost. We furthermore derive a topological invariant that shows a similar behavior.

TT 65.15 Wed 19:00 H 0104

Finite-temperature spectral functions: a Chebyshev-METTS approach — •Benedikt Bruognolo, Jan von Delft, and Andreas Weichselbaum — Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität, Munich

While nowadays a wide range of techniques exist to access the static and dynamic ground state properties of strongly correlated 1D quantum systems, finite-temperature calculations of such models still represent a challenge.

We introduce a new and efficient approach for calculating finite-temperature spectral functions directly in the frequency domain; it combines the Minimally Entangled Typical Thermal States (METTS) approach for thermal averaging with a double Chebyshev expansion for obtaining spectral information. We discuss the key steps of our method and its applicability in the context of the exactly solvable XX model. Moreover, we present preliminary results for an anisotropic spin-3/2 Heisenberg model with in-plane magnetic field.

TT 66: Superconductivity: Tunneling, Josephson Junctions, SQUIDs

Time: Wednesday 15:00–19:15 Location: H 2053

TT 66.1 Wed 15:00 H 2053

Coherent terahertz emission from $Bi_2Sr_2CaCu_2O_8$ intrinsic Josephson junction stacks — •Fabian Rudau[1], Boris Gross[1], Raphael Wieland[1], Nickolay Kinev[2], Manabu Tsujimoto[3], Min Ji[4,5], Ya Huang[4,5], Xianjing Zhou[4,5], Deyue An[4,5], Thomas Judd[1], Peiheng Wu[5], Takeshi Hatano[4], Huabing Wang[4,5], Valery Koshelets[2], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Physikalisches Institut and Center for Collective Quantum Phenomena in LISA$^+$, Universität Tübingen, Tübingen, Germany — [2]Kotel'nikov Institute of Radio Engineering and Electronics, Moscow, Russia — [3]Kyoto University, Kyoto, Japan — [4]National Institute for Materials Science, Tsukuba, Japan — [5]Research Institute of Superconductor Electronics, Nanjing University, Nanjing, China

Stacks of intrinsic Josephson junctions, made of the high temperature superconductor $Bi_2Sr_2CaCu_2O_8$, are promising candidates to be used as generators of electromagnetic waves in the terahertz regime, in principle allowing frequencies up to ∼10 THz. Ranging from 0.4 to 1 THz, coherent emission was detected from large, rectangular stacks, producing several tens of microwatt in power. Despite of several years of research, the mechanism of synchronizing all the junctions in the stack is still not fully understood. We investigated the heat distribution and electromagnetic standing waves in such stacks, as well as the generation of terahertz radiation, using a combination of electric transport measurements, direct radiation detection and low temperature scanning laser microscopy. Recent experimental results from our collaboration will be presented and compared to numerical simulations.

TT 66.2 Wed 15:15 H 2053

Multi-photon dressing of an anharmonic superconducting many-level quantum circuit — •Jochen Braumüller[1], Joel Cramer[1], Steffen Schlör[1], Hannes Rotzinger[1], Lucas Radtke[1], Alexander Lukashenko[1], Ping Yang[1], Sebastian Skacel[1], Sebastian Probst[1], Michael Marthaler[2], Lingzhen Guo[2], Alexey V. Ustinov[1,3], and Martin Weides[1] — [1]Karlsruhe Institute of Technology (KIT), Physikalisches Institut, 76131 Karlsruhe, Germany — [2]Karlsruhe Institute of Technology (KIT), Institut für Theoretische Festkörperphysik, 76131 Karlsruhe, Germany — [3]National University of Science and Technology MISIS, Moscow 119049, Russia

We report on the investigation of a superconducting anharmonic multilevel circuit that is coupled to a harmonic readout resonator. We observe multi-photon transitions via virtual energy levels of our system up to the fifth excited state. The back-action of these higher-order excitations on our readout device is analyzed quantitatively and demonstrated to be in accordance with theoretical expectation. By applying a strong microwave drive we achieve multi-photon dressing of our system which is dynamically coupled by a weak probe tone. The emerging higher-order Rabi sidebands and associated Autler-Townes splittings

involving up to five levels of the investigated anharmonic circuit are observed. Experimental results are in good agreement with master equation simulations.

TT 66.3 Wed 15:30 H 2053

Non-linear classical dynamics in a superconducting circuit containing a cavity and a Josephson junction — •Selina Meister, Björn Kubala, Vera Gramich, Michael Mecklenburg, Jürgen T. Stockburger, and Joachim Ankerhold — Institute for Complex Quantum Systems, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm, Germany

Motivated by recent experiments [1] a superconducting hybrid circuit consisting of a voltage biased Josephson junction in series with a resonator is studied. For strong driving the dynamics of the system can be very complex, even in the classical regime. Studying the dissipative dynamics within a Langevin-type description, we obtain well-defined dynamical steady states.

In contrast to the well-known case of anharmonic potentials, like the Duffing or parametric oscillator, in our case the non-linearity stems from the peculiar way the external drive couples to the system [2]. We investigate the resonance behaviour of this non-linear hybrid system, in particular when driving at higher- or subharmonics. The resulting down- and up-conversions can be observed both, as resonances in the I-V curve, and in the emitted microwave radiation, which yields additional spectral information.

[1] M. Hofheinz et al., PRL 106, 217005 (2011).
[2] V. Gramich et al., PRL 111, 247002 (2013).

TT 66.4 Wed 15:45 H 2053

Displacement of microwave squeezed states with Josephson parametric amplifiers — •Ling Zhong[1,2,3], Kirill Fedorov[1], Martin Betzenbichler[1,2], Stefan Pogorzalek[1,2], Alexander Baust[1,2,3], Edwar Xie[1,2,3], Max Haeberlein[1,2], Manuel Schwarz[1,2,3], Peter Eder[1,2], Jan Goetz[1,2], Karl Friedrich Wulschner[1,2], Edwin Menzel[1], Hans Hübl[1,2], Frank Deppe[1,2], Achim Marx[1], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 München, Germany

Propagating quantum microwaves are promising building blocks for quantum communication. Interestingly, such itinerant quantum microwaves can be generated in the form of squeezed photon states by Josephson parametric amplifiers (JPA). We employ a specific "dual-path" setup for both state reconstruction and JPA characterization. Displacement operations are performed by using a directional coupler after the squeezing. We compare our results with theory predictions. In particular, we discuss our experiments in the context of remote state preparation and quantum teleportation with propagating microwaves.

This work is supported by the DFG via SFB 631 and EU projects CCQED and PROMISCE.

TT 66.5 Wed 16:00 H 2053

The parity effect in a Jospehson junction array — Jared Cole[1], Andreas Heimes[2], and •Michael Marthaler[2] — [1]Chemical and Quantum Physics, School of Applied Sciences, RMIT University, Melbourne, Victoria 3001, Australia — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

We study transport in a Josephson junction array for small Josephson energies. For very small Josephson energy the transport is dominated by single quasiparticle tunneling. We consider a regime where there is enough energy to inject quasiparticles by breaking a cooper-pair, but transport inside of the array is dominated by the parity effect. This means that the current is caried by a small number of quasiparticles above the gap. We observer the crossover temperature T^*, which is also known from parity experiments in superconducting single electron transistors.

TT 66.6 Wed 16:15 H 2053

Even-odd flux quanta effect in the Fraunhofer oscillations of an edge-channel Josephson junction — •Benjamin Baxevanis, Viacheslav Ostroukh, and Carlo Beenakker — Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands

We calculate the beating of $h/2e$ and h/e periodic oscillations of the flux-dependent critical supercurrent through a quantum spin-Hall insulator between two superconducting electrodes [1]. A conducting pathway along the superconductor connects the helical edge channels via a non-helical channel, allowing an electron incident on the superconductor along one edge to be Andreev reflected along the opposite edge. We find the appearance of Fraunhofer oscillations with an even-odd effect: Large peaks in the critical current at even multiples of $h/2e$ alternate with smaller peaks at odd multiples. This even-odd effect has been recently observed in one series of experiments by Pribiag et al. [2].

[1] B. Baxevanis et al. arXiv:1411.6638
[2] V.S. Pribiag et al. arXiv:1408.1701

TT 66.7 Wed 16:30 H 2053

Experiments on phase retrapping in φ Josephson junctions — •Edward Goldobin[1], Rosina Menditto[1], Martin Weides[2], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]University of Tübingen, Tübingen, Germany — [2]KIT, Karlsruhe, Germany

We experimentally study retrapping of the phase in φ Josephson junctions (JJs) based on superconductor-insulator-ferromagnet-superconductor (SIFS) 0-π heterostructures[1,2]. Such φ JJs have a doubly degenerate ground state (two potential energy wells) with the phases $\pm\varphi$ ($0 < \varphi < \pi$). We study in which of these two wells the phase is trapped upon return of the JJ to the zero voltage state. We find that for $T > T^* \approx 2.4\,\mathrm{K}$ (large damping) the phase is always trapped in the $+\varphi$ state. However, for lower T (small damping) the trapping result is a statistical mixture of the $+\varphi$ and the $-\varphi$ states due to the presence of noise in the system. The probability for retrapping to the $-\varphi$ state increases and oscillates as T is decreasing below T^*, reaching a saturation value of $\sim 30\%$ for $T \lesssim 1.2\,\mathrm{K}$. These results are compared with theory[3], which predicts the butterfly effect in the limit of low damping.

[1] E. Goldobin et al. Phys. Rev. Lett. **107**, 227001 (2011).
[2] H. Sickinger et al. Phys. Rev. Lett. **109**, 107002 (2012).
[3] E. Goldobin et al. Phys. Rev. Lett. **111**, 057004 (2013).

TT 66.8 Wed 16:45 H 2053

Signatures of singlet-triplet pairing in Josephson transport between a conventional and a noncentrosymmetric superconductor — Björn Sothmann[1] and •Rakesh Tiwari[2] — [1]Département de Physique Théorique, Université de Genève , CH-1211 Genève 4, Switzerland — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

We investigate Josephson response of a junction consisting of a noncentrosymmetric superconductor tunnel coupled to a conventional s-wave superconductor via a double quantum dot. In the presence of an inhomogenous magnetic field acting on the two quantum dots forming the double quantum dot, the current phase relationship becomes highly asymmetric. The asymmetry in the critical current can be used to quantify the triplet-singlet pairing ratio in the noncentrosymmetric superconductor.

15 min. break.

Invited Talk TT 66.9 Wed 17:15 H 2053

Probing Andreev Bound States in One-Atom Superconducting Contacts — •Hugues Pothier, Camille Janvier, Leandro Tosi, Çağlar Girit, Marcelo Goffman, Daniel Esteve, and Cristiàn Urbina — Quantronics Group, SPEC, CEA-Saclay, France

Superconductors are characterized by a dissipationless current. Since the work of Josephson 50 years ago, it is known that a supercurrent can even flow through tunnel junctions between superconductors. This Josephson effect also occurs through any type of "weak links" between superconductors: non-superconducting materials, constrictions, ... A unified understanding of the Josephson effect has emerged from a mesoscopic description of weak links. It relies on the existence of doublets of localized states that have energies below the superconducting gap: the Andreev bound states. I will present experiments performed on the simplest conductor possible, a single-atom contact between superconductors, that illustrate these concepts. The most recent work demonstrates time-domain manipulation of quantum superpositions of Andreev bound states.

TT 66.10 Wed 17:45 H 2053

Superconducting phase transition in STM tips — •Matthias Eltschka[1], Berthold Jäck[1], Maximilian Assig[1], Markus

Etzkorn[1], Christian R. Ast[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The superconducting properties of systems with dimensions comparable to the London penetration depth considerably differ from macroscopic systems. We have studied the superconducting phase transition of vanadium STM tips in external magnetic fields. Employing Maki's theory we extract the superconducting parameters such as the gap or the Zeeman splitting from differential conductance spectra. While the Zeeman splitting follows the theoretical description of a system with $s = 1/2$ and $g = 2$, the superconducting gaps as well as the critical fields depend on the specific tip. For a better understanding of the experimental results, we solve a one dimensional Usadel equation modeling the superconducting tip as a cone with the opening angle α in an external magnetic field. We find that only a small region at the apex of the tip is superconducting in high magnetic fields and that the order of the phase transition is directly determined by α. Further, the spectral broadening increases with α indicating an intrinsic broadening mechanism due to the conical shape of the tip. Comparing these calculations to our experimental results reveals the order of the superconducting phase transition of the STM tips.

TT 66.11 Wed 18:00 H 2053

Dynamics of a nanoscale Josephson junction probed by scanning tunneling microscopy — •Christian R. Ast[1], Berthold Jäck[1], Matthias Eltschka[1], Markus Etzkorn[1], and Klaus Kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]Institut de Physique de la Matière Condensée, EPFL, Lausanne

The Josephson effect is an intriguing phenomenon as it presents an interplay of different energy scales, such as the Josephson energy ϵ_J (critical current), charging energy ϵ_C, and temperature T. Using a scanning tunneling microscope (STM) operating at a base temperature of 15 mK, we create a nanoscale superconductor-vacuum-superconductor tunnel junction in an extremely underdamped regime ($Q \gg 10$). We observe extremely small retrapping currents also owing to strongly reduced ohmic losses in the well-developed superconducting gaps. While formally operating in the zero temperature limit, i. e. the temperature T is smaller than the Josephson plasma frequency ω_J ($k_B T \ll \hbar\omega_J = \sqrt{8\epsilon_J\epsilon_C}$), experimentally other phenomena, such as stray photons, may perturb the Josephson junction, leading to an effectively higher temperature. The dynamics of the Josephson junction can be addressed experimentally by looking at characteristic parameters, such as the switching current and the retrapping current. We discuss the dynamics of the Josephson junction in the context of reaching the zero temperature limit.

TT 66.12 Wed 18:15 H 2053

Supersymmetry in a Cooper-pair box shunted by a Josephson rhombus — •Jascha Ulrich, Daniel Otten, and Fabian Hassler — JARA-Institute for Quantum Information, RWTH Aachen University

Recently, a new kind of quantum-mechanical supersymmetry has been proposed providing a generalization of supersymmetry of the free particle to the presence of a periodic potential. Here, we propose a physical realization in a Cooper-pair box shunted by an effectively pi-periodic Josephson junction rhombus. For a characteristic ratio between the strength of the 2pi- and the pi-periodic junction, this yields a degeneracy of the energy levels all the way from the weak junction/charge qubit limit to the strong junction/transmon regime. We give explicit results for the required rhombus parameters as a function of the conventional junction strength and show that tuning in and out of the supersymmetric point is easily achieved by varying the junction strength or an external gate voltage. We furthermore discuss a microwave experiment for level spectroscopy and conclude that the supersymmetry could indeed be realized with currently existing Josephson junction technology.

TT 66.13 Wed 18:30 H 2053

Dynamical phase squeezing in layered superconductors (limit of two coupled junctions) — •Beilei Zhu[1], Robert Höppner[1], Tobias Rexin[1], Andrea Cavalleri[1,2,3], and Ludwig Mathey[1,4] — [1]ZOQ & ILP, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]MPI for Structure and Dynamics of Matter, 22761 Hamburg, Germany — [3]Clarendon Laboratory,Department of Physics, Oxford University, Parks Road, Oxford OX1 3PU,UK — [4]The Hamburg Center for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

We study the dynamics of a layered superconductor with alternating inter-layered coupling, driven by an external potential that models a light pulse coupling to an optical phonon mode, inspired by [1,2]. We study a minimal model consisting of one strong junction and one weak junction, coupled to a heat bath. We describe this toy model using a Langevin formalism and treat it numerically. The strong junction plays as an amplifier of the external driving on the weak junction. We find that the phase fluctuations of the weak junction are squeezed under near-resonant driving of strong junction. The power spectrum demonstrates that the squeezing occurs in the low frequency regime. We also consider a quantum version for a driven single Josephson Junction.

[1] Fausti et al., Science, 331, 6014 189-191 (2011)
[2] Kaiser et al., arXiv:1205.4661

TT 66.14 Wed 18:45 H 2053

Redistribution of phase fluctuations in a periodically driven cuprate superconductor — •Robert Höppner[1], Beilei Zhu[1], Tobias Rexin[1], Ludwig Mathey[1,4], and Andrea Cavalleri[2,3] — [1]Zentrum für Optische Quantentechnologien und Institut für Laserphysik, Hamburg, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [3]Department of Physics, Oxford University, Clarendon Laboratory, Parks Road, Oxford, UK — [4]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

We study the thermally fluctuating state of a bi-layer cuprate superconductor under the periodic action of a staggered field oscillating at optical frequencies. This analysis distills essential elements of the recently discovered phenomenon of light enhanced coherence in YBCO, which was achieved by periodically driving infrared active apical oxygen distortions. The effect of a staggered periodic perturbation is studied using a Langevin description of driven, coupled Josephson junctions, which represent two neighboring pairs of layers and their two plasmons. We demonstrate that the external driving leads to a suppression of phase fluctuations of the low-energy plasmon, an effect which is amplified via the resonance of the high energy plasmon, with a striking suppression of the low-energy fluctuations, as visible in the power spectrum. We also find that this effect acts onto the in-plane fluctuations, which are reduced on long length scales and we discuss the behavior of vortices in the ab-planes and across the weakly coupled junctions.

TT 66.15 Wed 19:00 H 2053

Dynamics of a driven Josephson junction at high temperature — •Tobias Rexin[1,2,3], Beilei Zhu[1,2,3], Robert Hoeppner[1,2,3], and Ludwig Mathey[1,2,3,4] — [1]Uni Hamburg — [2]Institut für Laserphysik Hamburg — [3]Zentrum für optische Quantentechnologien — [4]Center for Ultrafast Imaging

The present work investigates the dynamics of a single driven Josephson junction coupled to a thermal bath. Applying an extended version of the Fokker-Planck equation, namely the Kramers equation, we analytically treat the dynamics of both degrees of freedom the phase and the charge density. Interestingly, instead of heating the junction, the driving can suppress the phase fluctuations [1]. This is motivated by recent pump-probe experiments of high T_c superconductors reported in [2,3]. In ref [1], we have developed a description of the dynamics in these materials by modeling them as an array of Josephson junctions. The single junction model is a simplification of the Josephson junction array, which already exhibits qualitative aspects of the driven array.

[1] R.Höppner et al. *preprint* arXiv:1406.3609v2
[2] W. Hu, et al., *Nature Materials* **13**, 705 (2014).
[3] S. Kaiser, et al. *Phys. Rev. B* **89**, 184516 (2014).

TT 67: Correlated Electrons: f-Electron Systems

Time: Wednesday 15:00–17:45 Location: H 3005

TT 67.1 Wed 15:00 H 3005

Electronic Structure and Core-Level Spectroscopy of Light Actinide Dioxides — •Jindrich Kolorenc — Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

The correlated band theory implemented as a combination of the local density approximation with the dynamical mean-field theory (LDA+DMFT) is applied to UO_2, NpO_2, and PuO_2 [1]. The calculated band gaps and valence-band spectra are in very good agreement with optical absorption measurements and with experimental photoemission spectra. The relatively large hybridization of the actinide 5f shell with the p states of oxygen causes a sizable increase of the filling of the 5f orbitals from the nominal ionic configurations with 2, 3, and 4 electrons to fractional values 2.5, 3.4, and 4.4. This enhancement is compatible with the 4f core-level photoemission spectra [2] but in the same time it appears to disagree with the recent synchrotron experiments employing the resonant x-ray emission spectroscopy (RXES) [3,4]. The discrepancy will be analyzed in the LDA+DMFT framework.

[1] A. B. Shick, J. Kolorenc, L. Havela, T. Gouder, and R. Caciuffo, Phys. Rev. B **89**, 041109(R) (2014).
[2] A. Kotani and T. Yamazaki,
Prog. Theor. Phys. Suppl. **108**,117 (1992).
[3] K. O. Kvashnina, Y. O. Kvashnin, and S. M. Butorin,
J. Electron. Spectrosc. Relat. Phenom. **194**, 27 (2014).
[4] C. H. Booth (private communication).

TT 67.2 Wed 15:15 H 3005

$GdRh_2Si_2$: Single crystal growth and characterization — •Kristin Kliemt and Cornelius Krellner — Physikalisches Institut, Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany

Among the ternary silicides of the type RT_2Si_2 (R = rare earth, T = transition metal) which crystallize in the bodycentered tetragonal $ThCr_2Si_2$ structure, $GdRh_2Si_2$ has attracted much attention in the last decades [1,2] as it belongs to the compounds with rare earth elements with exceptional magnetic properties e.g. $CeRh_2Si_2$, $YbRh_2Si_2$ and $EuRh_2Si_2$. Single crystals of $GdRh_2Si_2$ were grown for the first time by a modified Bridgman method from indium flux.

We report on the growth procedure and show the results of specific heat, magnetic and electrical transport measurements on the single crystals. The high quality of the crystals was proved by Laue X-ray scattering, X-ray powder diffraction, EDX microprobe analysis and resistivity measurements.

[1] I. Felner, I. Nowik, Solid State Commun. **47**, 831 (1983).
[2] G.A. Cabrera-Pasca *et al.*,
J. Phys. Condens. Matter **24**, 416002 (2012).

TT 67.3 Wed 15:30 H 3005

Measuring the T-dependence of the penetration depth of $CeCu_2Si_2$ with superconducting microwave resonators at mK temperatures — •Markus Thiemann[1], Martin Dressel[1], Marc Scheffler[1], Silvia Seiro[2], Christoph Geibel[2], and Frank Steglich[2] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

Microwave measurements on superconductors can reveal the temperature dependence of the penetration depth, which can indicate the presence of nodes in the superconducting gap function. $CeCu_2Si_2$ is a heavy-fermion superconductor with critical temperature $T_c \approx 0.6$ K. Though $CeCu_2Si_2$ for a long time was believed to be a d-wave superconductor, at present it is under debate whether its order parameter features nodes or not.

Therefore, we have performed microwave measurements to study the penetration depth, but we address the microwave surface resistance as well. To be able to probe superconducting bulk samples at mK temperature, we have developed a new experimental approach based on superconducting stripline resonators. We evaluate the performance of this technique at temperatures down to 30 mK by studying the conventional superconductor zirconium (T_c similar to that of $CeCu_2Si_2$). Comparing our data on the penetration depth of a $CeCu_2Si_2$ single crystal with that of zirconium, we find a clear difference in the temperature dependence, which we discuss in terms of possible nodes or multiband superconductivity.

TT 67.4 Wed 15:45 H 3005

Elastic Response of URu_2Si_2 under High Magnetic Fields — •Tatsuya Yanagisawa[1], Shota Mombetsu[1], Hiroyuki Hidaka[1], Hiroshi Amitsuka[1], Mitsuhiro Akatsu[2], S. Yasin[3], S. Zherlitsyn[3], J. Wosnitza[3], K. Huang[4], M. Janoschek[4], and M. B. Maple[4] — [1]Dept. of Physics, Hokkaido Univ., Sapporo, Japan — [2]Grad. School of Science and Technology, Niigata Univ., Niigata, Japan — [3]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf and TU Dresden, Dresden, Germany — [4]Dept. of Physics, Univ. of California, San Diego, La Jolla, U.S.A.

We have measured the elastic constants, C_{44}, C_{66}, $(C_{11} - C_{12})/2$ in URu_2Si_2 by means of high-frequency ultrasonic measurements in pulsed magnetic fields up to 68.7 T in a wide temperature range from 1.5 to ∼120 K. We found a reduction of $(C_{11} - C_{12})/2$ for magnetic field $H \parallel [001]$ that appears only in the temperature and magnetic field region in which URu_2Si_2 exhibits a heavy-electron state and hidden order. This change in $(C_{11} - C_{12})/2$ appears to be a response of the $5f$ electrons to an orthorhombic and volume conservative strain field $\varepsilon_{xx} - \varepsilon_{yy}$ with Γ_3 symmetry. The lattice instability is likely related to a symmetry-breaking band instability that arises due to the hybridization of the localized $5f$ electrons with the conduction electrons and is probably linked to the hidden-order parameter of this compound. Recent progress obtained by our measurements of the transverse ultrasonic modes C_{44} and C_{66} will also be discussed.

Two of the authors (T.Y. & S.M.) are supported by the Strategic Young Researcher Overseas Visits Program for Accelerating Brain Circulation from the JSPS.

TT 67.5 Wed 16:00 H 3005

Magnetic and transport properties of structural variants of Remeika phases: $Th_3Ir_4Ge_{13}$ and $U_3Ir_4Ge_{13}$ — •Roman Gumeniuk[1,2], Walter Schnelle[1], Andreas Leithe-Jasper[1], and Yuri Grin[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09596 Freiberg, Germany

$Th_3Ir_4Ge_{13}$ and $U_3Ir_4Ge_{13}$ crystallize with primitive cubic $Tm_3Co_4Ge_{13}$ and non-centrosymmetric rhombohedral HT-$Y_3Pt_4Ge_{13}$ type of structures, respectively, which are derivatives of the cubic $Yb_3Rh_4Sn_{13}$ prototype. Measurements of magnetic susceptibility, electrical resistivity, specific heat, thermopower, and thermal conductivity reveal, that $Th_3Ir_4Ge_{13}$ is a diamagnetic bad metal and undergoes a first-order phase transition at ≈ 200 K. Charge-density wave (CDW) and structural phase-transition scenarios for $Th_3Ir_4Ge_{13}$ are discussed. $U_3Ir_4Ge_{13}$ is Curie-paramagnetic ($\mu_{\text{eff}} = 4.05\ \mu_B$) and orders ferromagnetically at $T_C = 15$ K. The U $5f$ electrons in $U_3Ir_4Ge_{13}$ are predominantly of itinerant nature.

TT 67.6 Wed 16:15 H 3005

Magnetic order in CeAuSn — •O. Stockert[1], M-H. Lémée-Cailleau[2], C. L. Huang[1,3], Z. Huesges[1], S. Lucas[1], V. Fritsch[3,4], and H. v. Löhneysen[3] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Germany — [4]Institut für Physik, Universität Augsburg, Augsburg, Germany

CeAuSn is a hexagonal, rare-earth based intermetallic compound exhibiting antiferromagnetic order below $T_N = 4.1$ K as evidenced by anomalies in thermodynamic properties. In order to study the magnetic order using a microscopic probe, neutron diffraction was performed on a CeAuSn single crystal. Diffraction pattern were recorded using the neutron Laue diffractometer CYCLOPS at ILL. Allowing fast exploration of reciprocal space, this innovative instrument only recently became available for users. Data were taken at temperatures between $T = 1.6$ and 10 K. Our measurements confirm the hexagonal crystal structure at low temperatures and additional magnetic peaks are clearly visible at lowest temperatures. They can be indexed by a commensurate propagation vector $k = (1/2\ 0\ 0)$. Moreover, the magnetic intensity vanishes at $T_N \approx 4.1$ K in line with thermodynamic measurements. Although CeAuSn is an XY system on a triangular

lattice where geometrical frustration might play a role, we do not find evidence for the existence of frustration.

15 min. break.

TT 67.7 Wed 16:45 H 3005

Multiple magnetic-field-induced transitions in the Kondo lattice $YbNi_4P_2$ — •Heike Pfau[1], Ramzy Daou[2], Alexander Steppke[1], Dan Sun[1], Kristin Kliemt[3], Cornelius Krellner[3], Christoph Geibel[1], Frank Steglich[1], and Manuel Brando[1] — [1]Max-Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Laboratoire CRISMAT, UMR 6508 du CNRS, ENSICAEN et Université de Caen, F-14050 Caen, France — [3]Institute of Physics, Goethe University Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany

$YbNi_4P_2$ is a ferromagnetic Kondo lattice system with a Kondo temperature of 8K and a small Curie temperature of 0.15K. It is close to a ferromagnetic quantum critical point, which can be induced by substitution of phosphorus by arsenic. A magnetic field of 60mT applied along the crystallographic *c*-axis is also able to suppress the ferromagnetic order, above which $YbNi_4P_2$ is a field-polarized Fermi liquid. We performed thermopower, resistivity, and specific heat measurements to study the evolution of $YbNi_4P_2$ in magnetic fields up to 12T. While we observe signatures of strong fluctuations at small fields, our measurements detect multiple transitions at higher fields between 2T and 12T. To analyse this high field behaviour, we compare our results to previous studies on the two Kondo lattices $YbRh_2Si_2$ and $CeRu_2Si_2$.

TT 67.8 Wed 17:00 H 3005

Momentum-space structure of quasielastic spin fluctuations in $Ce_3Pd_{20}Si_6$ — •P. Y. Portnichenko[1], A. S. Cameron[1], M. A. Surmach[1], P. P. Deen[2,3], S. Paschen[4], A. Prokofiev[4], J.-M. Mignot[5], A.M. Strydom[6], M.T.F. Telling[7,8], A. Podlesnyak[9], and D. S. Inosov[1] — [1]TU Dresden, Germany — [2]ESS, Sweden — [3]Univ. of Copenhagen, Denmark — [4]Vienna Univ. of Technology, Austria — [5]LLB, France — [6]Univ. of Johannesburg, South Africa — [7]ISIS, UK — [8]Univ. of Oxford, UK — [9]SNS, USA

Among heavy-fermion metals, $Ce_3Pd_{20}Si_6$ is one of the heaviest-electron systems known to date. Using high-resolution neutron spectroscopy, we observed low-energy magnetic scattering from a single crystal of this compound in the paramagnetic state. We investigated its temperature dependence and distribution in **Q** space. At low temperatures, a quasielastic magnetic response persists with varying intensity all over the Brillouin zone. It forms a broad hump centered at the (111) scattering vector, surrounded by minima of intensity at (002), (220) and equivalent wave vectors. The **Q**-space structure distinguishes this signal from a simple crystal-field excitation and rather lets us ascribe it to short-range dynamical correlations between the neighboring Ce ions, mediated by the itinerant heavy *f*-electrons via the RKKY mechanism. Upon heating, the energy width of the signal follows the conventional $T^{1/2}$ law, $\Gamma(T) = \Gamma_0 + A\sqrt{T}$. The **Q**-space symmetry of the quasielastic response suggests that it stems from the simple-cubic Ce sublattice occupying the 8c Wyckoff site, whereas the inequivalent 4a site remains magnetically silent.

TT 67.9 Wed 17:15 H 3005

Ambient pressure superconductivity emerging in the antiferromagnetic phases of the novel heavy fermion compounds Ce_3PdIn_{11} and Ce_3PtIn_{11} — •Marie Kratochvílová, Jan Prokleška, Klára Uhlířová, Vladimír Sechovský, and Jeroen Custers — Department of Condensed Matter Physics, Charles University, Prague, Ke Karlovu 5, 121 16, Czech Republic

$Ce_nT_mIn_{3n+2m}$ (n=1,2; m=1; T=transition metal) heavy fermion compounds are known to be on the verge of a magnetic to non-magnetic quantum critical point (QCP). In close vicinity of the QCP they exhibit an unconventional superconducting state. However, this family of compounds is interesting for an other reason. The compounds crystallize in the tetragonal structures which provide the possibility to tune the structural dimensionality from more 2D to 3D (stoichiometries: 115-218-103). This makes them ideal candidates to investigate the influence of the parameter dimensionality with respect to quantum criticality.

Ce_3TIn_{11} (T=Pd,Pt) single crystals were prepared for the first time. Ce_3PtIn_{11} (Ce_3PdIn_{11}) exhibits two successive transitions at T_1=2.2K (T_1=1.7K) and T_N=2.0K (T_N =1.5K) into incommensurate and commensurate local moment antiferromagnetic states, respectively. Applying magnetic field along the c-axis gradually suppresses both transitions; they merge at 4T and split again in higher fields. Superconductivity emerges at T_C=0.32K (T_C=0.39K) and it is enhanced by the application of hydrostatic pressure. The unusual magnetic phase diagram will be discussed in the context of superconductivity and magnetism in related compounds.

TT 67.10 Wed 17:30 H 3005

Charge fluctuations and coherence in the mixed-valence regime investigated on $Sm_{1-x}La_xB_6$ — •Chul-Hee Min[1], Kuang-Shing Chen[2], Hendrik Bentmann[1], Sebastian Fiedler[1], Boyoun Kang[3], Beongki Cho[3], Jan Werner[2], Fahker Assaad[2], and Friedrich Reinert[1] — [1]Universität Würzburg, EP7, Würzburg, Germany — [2]Universität Würzburg, TP1, Würzburg, Germany — [3]School of Materials Science and Engineering, Gwangju Institute of Science and Technology (GIST), Gwangju, Korea.

We present an investigation on the temperature dependence of $4f$ states and $3d$ core-levels in $Sm_{1-x}La_xB_6$ in order to identify the unique electronic properties of a mixed valence regime. By use of photon energies from VUV to hard x-rays (HAXPES), we separate surface and bulk properties, which show significant differences. Our results particularly by HAXPES indicate that charge fluctuations in SmB_6 are a rather local property, which might influence the expectation value of the potential energy. A characteristic feature and the signature of the lattice coherence in a mixed valence regime will be demonstrated and discussed.

TT 68: Correlated Electrons: (General) Theory 1

Time: Wednesday 15:00–18:15 Location: H 3010

TT 68.1 Wed 15:00 H 3010

Ab-initio study of the finite temperature magnetism in iron and nickel — Michael Karolak[1], •Andreas Hausoel[1], Ersoy Sasioglu[2], Alessandro Toschi[3], Andrey A. Katanin[4], Karsten Held[3], Alexander Lichtenstein[5], and Giorgio Sangiovanni[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [2]Peter Grünberg Institut, Forschungszentrum Jülich — [3]Institute of Solid State Physics, TU Wien — [4]Institute of Metal Physics, Ekaterinburg — [5]Institut für Theoretische Physik, Universität Hamburg

The calculation of the ferromagnetic transition temperature of itinerant ferromagnets like iron and nickel has been a very hard problem for theory ever since. This is due to the interplay between strong local interactions and the itinerant character of the electrons. Here we show fully ab-initio DFT+DMFT calculations for bcc-iron and fcc-nickel, using the numerically exact Continuous Time Quantum Monte Carlo method in hybridization expansion. We consider the full cubic Coulomb interaction from cRPA and discuss the effects of different commonly used approximations, i.e. density-density and Slater-Kanamori. This way we obtain the best ab-initio estimates of the transition temperatures of iron and nickel one can achieve with static interactions and neglecting non-local spatial correlations.

TT 68.2 Wed 15:15 H 3010

La_2NiTiO_6: A 3D $S = 1$ fcc Heisenberg antiferromagnet — Michael Karolak, •Martin Edelmann, and Giorgio Sangiovanni — Institut für Theoretische Physik und Astrophysik, Universität Würzburg

The double perovskite La_2NiTiO_6 is identified as an interesting $S = 1$ quantum antiferromagnet on a three-dimensional fcc sublattice. By means of Density Functional Theory (DFT) in combination with Dynamical Mean Field Theory (DMFT) it is demonstrated that this material is a high-spin *d*-electron system deep in the Heisenberg limit and established that its paramagnetic Mott phase persists down to low temperatures not because of frustration effects but rather for the strong coupling physics. The strong-coupling nature is assessed from a

multi-orbital DFT+DMFT analysis of the energetic balance between the ordered and disordered phase, which reveals a kinetic-energy-driven ordering. La_2NiTiO_6 emerges thus as a paradigmatic realization of a spin-triplet Mott insulator[1].

[1] M. Karolak, M. Edelmann, and G. Sangiovanni, arXiv:1407.2255 (2014).

TT 68.3 Wed 15:30 H 3010

Multi-orbital GW+(E)DMFT investigation of strongly correlated materials — •Lewin Boehnke[1], Fredrik Nilsson[2], Ferdi Aryasetiawan[2], and Philipp Werner[1] — [1]University of Fribourg, Switzerland — [2]Lund University, Sweden

The merits of the combination of the GW-formalism for non-local self-energy effects and (extended) dynamical mean field theory (E)DMFT to rigorously incorporate local fluctuations have been realized more than a decade ago [1], yet the numerical obstacles finding physically sound approximations for the respective parts prevented a broad adaption.

Previous approaches a GW+(E)DMFT treatment of strongly correlated multi-orbital electron systems employed various degrees of approximation for the DMFT impurity problem, the self-consistency and the interface of the two complementary methods.

We use suitable continuous time (CT-Hyb) solvers to deal with the frequency dependance of the impurity interaction and a fitted Matsubara-axis formulation of the GW-algorithm to examine the multi-orbital perspective to material investigations.

[1] Biermann, Aryasetiawan, Georges, PRL **90** (2003)

TT 68.4 Wed 15:45 H 3010

Electron correlation at the interface : A charge self-consistent DFT+DMFT approach. — •Sumanta Bhandary[1], Zhicheng Zhong[2], Liang Si[1], and Karsten Held[1] — [1]Institute of Solid State Physics, Vienna University of Technology, A-1040 Vienna, Austria — [2]Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We have employed a method to describe the interplay between structural distortion and induced charge as well as orbital degrees of freedom in a self-consistent way by combining density functional theory (DFT) and dynamical mean field theory (DMFT)[1]. The scheme involves solution of the full system in a local density approximation (Wien2K) followed by a wannier projection on correlated sub-bands (Wannier90). The impurity problem is treated with DMFT by employing continuous time quantum monte carlo (CT-QMC) method in the hybridization expansion (w2dynamics). The correlation induced correction to the charge density is incorporated in the total charge, which is obtained over a self-consistent loop of DFT and DMFT. The thin layer of $SrVO_3$ (SVO) on $SrTiO_3$ (STO) undergoes a Mott-Hubbard transition due to the spontaneous orbital symmetry breaking [2]. In contrast to SVO, there is a significant charge transfer between the layers of $SrRuO_3$.

We acknowledge financial support from European Research Council under (FP/2007- 2013)/ERC through grant agreement n. 306447 (JT,KH).

[1] F. Lechermann *et al.* PRB 74, 125120;
L. V. Pourovskii *et al.* PRB 76, 235101.
[2] Z. Zhong *et al.* arXiv:1312.5989.

TT 68.5 Wed 16:00 H 3010

Charge self-consistent DFT+Many-body with a flexible self-energy representation — •Christoph Piefke, Malte Behrmann, and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany

Starting from ab initio density functional theory in its local density approximation (DFT/LDA), strongly correlated electron systems are investigated using a combination of different self-energy approximations in a charge-self-consistent approach. After identifying a correlated subspace via projections onto localized orbitals [1], a multi-orbital Hubbard-Hamiltonian, including spin-flip-, pair-hopping- and spin-orbit-coupling-terms, is introduced. Fed with parameters from experiment, this operator gives rise to a self-energy-correction, which can be treated in different approximations, e.g. by taking it as the orbital occupation times interaction strength (Hartree-Fock, HF) or by mapping the interactions onto an itinerant quasiparticle part and localized bosonic degrees of freedom (e.g. Rotationally Invariant Slave-Boson Mean-Field theory, RISB-MF [2,3]). The correction flows back to LDA. We report, how this approach fits in the landscape of available techniques for strongly correlated electron systems and explore its chances and limits in the context of realistic strongly correlated materials.

[1] B. Amadon, F. Lechermann, A. Georges, F. Jollet, T.O. Wehling, and A.I. Lichtenstein, PRB **77**, 205112, (2008)
[2] T. Li, P. Wölfle, and P. J. Hirschfeld, PRB **40**, 6817 (1989)
[3] F. Lechermann, A. Georges, G. Kotliar, and O. Parcollet, PRB **76**, 155102, (2007)

TT 68.6 Wed 16:15 H 3010

Optimal bath discretization for exact diagonalization solvers of Anderson impurity models — •Malte Schüler[1,2], Christian Renk[1,2], and Tim Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, D-28359 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany

Exact diagonalization (ED) solvers of the Anderson impurity model (AIM) provide access to real frequency spectral properties and work in presence of arbitrarily complex Coulomb interactions, spin-orbit coupling and at low temperatures. Due to Hilbert space constrains the non-interacting bath of the AIM has however to be discretized, which is the main approximation within ED approaches and gives rise to ambiguities. We present a method which finds optimal parameters of the discretized model. Optimal means that the resulting density matrix represents the density matrix of the full model as closely as possible. This is accomplished by using a variational principle. We show benchmark results and comparisons to other discretization schemes and solvers like CT-QMC as well as first results on realistic 5-Orbital impurity models. Orbital occupancies, local spin moments and thermodynamic properties are well described within this variational ED approach.

15 min. break.

Topical Talk TT 68.7 Wed 16:45 H 3010

Structural Stability and Lattice Dynamics of Correlated Electron Materials — •Ivan Leonov — TP III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

I will discuss a computational scheme for the investigation of complex correlated electron materials which is able to treat atomic displacements, and hence structural transformations, caused by electronic correlations. It combines ab initio band structure and dynamical mean-field theory and is implemented in terms of plane-wave pseudopotentials. This approach is employed to compute the electronic structure and phase stability of several correlated electron materials. In particular, we study the cooperative Jahn-Teller effect in paramagnetic $KCuF_3$, the electronic properties and lattice dynamics of Fe at the bcc-fcc phase transition as a function of temperature, the electronic state and structural stability of V_2O_3 at the Mott-Hubbard metal-insulator transition, and the electronic structure and phase stability of FeSe. Our results for the equilibrium crystal structure, phase stability, and lattice dynamics are in quantitative agreement with experimental data. We find that electronic correlations are important to explain the lattice stability of correlated materials. We also present our recent results obtained by the LDA+DMFT approach implemented with the linear-response formalism regarding atomic displacements which makes it possible to evaluate the interatomic forces and, thereby, determine the atomic displacements. Our results show an overall good agreement between the total energy and force computations of the equilibrium atomic positions.

TT 68.8 Wed 17:15 H 3010

Correlated metal - Mott insulator heterostructures: real space dynamical mean-field study — •Karol Makuch and Krzysztof Byczuk — Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

Motivated by recent experiments on transition metal oxide interfaces we study models of heterostructures with strong electronic correlations. In particular, we investigate a layer of a Mott insulator sandwiched between two semi-infinite correlated metals. The width of a layer varies from one to many lattice constants. The system is described by the Hubbard model on a simple cubic lattice with the position dependent Hubbard interaction. Properties of the system are investigated within the real space dynamical mean-field theory with the continuous time quantum Monte Carlo solver created in our group. Proximity effects and structures of local excitations in different parts of the system are described.

TT 68.9 Wed 17:30 H 3010

Fluctuation diagnostics of the electron self-energy: Origin of the pseudogap physics — Olle Gunnarsson[1], Thomas Schäfer[2], James Le Blanc[3,4], Emanuel Gull[4], Jaime Merino[5], Giorgio Sangiovanni[6], Georg Rohringer[2], and •Alessandro Toschi[2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]IFP, Vienna University of Technology, Austria — [3]Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany — [4]Department of Physics, University of Michigan, Ann Arbor, USA — [5]Departamento de Física Teórica de la Materia Condensada, IFIMAC Universidad Autónoma de Madrid, Spain — [6]Institute of Physics and Astrophysics, University of Würzburg, Germany

We demonstrate how to identify which physical processes dominate the low-energy spectral functions of correlated electron systems. We obtain an unambiguous classification by analysing the equation of motion for the electron self-energy in its charge, spin and particle-particle representations. Our procedure is then employed to clarify the controversial physics responsible for the appearance of the pseudogap in correlated systems. We illustrate our method by examining the attractive and repulsive Hubbard model in two-dimensions. In the latter, spin fluctuations are identified as the origin of the pseudogap, and we also explain why *d*-wave pairing fluctuations play a marginal role in suppressing the low-energy spectral weight, independent of their actual strength.

TT 68.10 Wed 17:45 H 3010

Excitonic condensation of strongly correlated electrons — •Jan Kunes — Institute of Physics, ASCR, Prague, Czechia

Instabilities of the two-band Hubbard model in the vicinity of the spin-state transition are investigated using the dynamical mean-field theory. Excitonic condensation is found to be the leading instability in a part of the parameter space [1]. The complex nature of the exitonic order parameter allows several phases to be realised. We show that by doping away from half-filling all the symmetry allowed phases can be realised and investigate their physical properties [2,3].

[1] J. Kunes and P. Augustinsky, Phys. Rev. B 89, 115134 (2014)
[2] J. Kunes and P. Augustinsky, arXiv:1405.1191
[3] J. Kunes, arXiv:1410.5198

TT 68.11 Wed 18:00 H 3010

Dynamical electronic correlations in nanostructures — •Angelo Valli[1,2], Giorgio Sangiovanni[3], Alessandro Toschi[2], Massimo Capone[1], and Karsten Held[2] — [1]Democritos National Simulation Center, Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali (IOM) and Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy — [2]Vienna University of Technology, Vienna, Austria — [3]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany

The understanding and control of strong electronic correlation effects represents one of the most challenging research topic of modern solid state physics. Thanks to the refined ability to manipulate matter down to the nanoscale, we are nowadays able to explore electronic correlations within an artificial experimental environment. Moreover, the intrinsic high tunability of nano- and heterostructures hints at the fascinating possibility to directly control quantum phenomena. The experimental progress call for a deeper understanding of many-body effects on the nanoscale beyond paradigmatic models. To this end, we employ state-of-the art many-body methods within the reference frame of the dynamical mean-field theory and its extensions, in order to describe electronic, magnetic, and transport properties of nanoscopic systems. Among the applications, we explore the role of dynamical electronic correlations in carbon-based systems, ranging from few atoms molecules to graphene nanoflakes.

TT 69: Other Low Temperature Topics: Cold Atomic Gases

Time: Wednesday 15:00–19:00 Location: A 053

TT 69.1 Wed 15:00 A 053

Strongly Correlated Phases and Ferromagnetic Phases of Fermions in an Optical Flux Lattice Model — •Simon Davenport and Nigel Cooper — Cavendish Laboratory, 19 J J Thomson Avenue, Cambridge, CB3 0HE

We study a theoretical model of a 2-dimensional ultracold atomic gas subject to an "optical flux lattice": a particular laser configuration where Raman-dressed atoms experience a strong effective magnetic field, which can lead to a bandstructure of narrow energy bands with non-zero Chern numbers. In this optical flux lattice we place spin-1/2 fermions that interact via a Feshbach-resonance induced contact interaction, coupling spin-up and spin-down particles. Atoms restricted to the lowest band are described by an effective model of spinless fermions with a tunable interaction coupling states in a momentum-dependent manner across the Brillouin zone. This non-local interaction is due to the Raman coupling between spin-up and spin-down levels. We present a summary of results from a detailed exact diagonalization study of the effective lowest band model. In particular we offer evidence indicating the presence of strongly correlated phases and ferromagnetic phases.

TT 69.2 Wed 15:15 A 053

Ground states for the Bose-Hubbard model with flat bands — •Petra Pudleiner[1] and Andreas Mielke[2] — [1]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [2]Institute for Theoretical Physics, Ruprecht-Karls University, Heidelberg, Germany

Flat band systems have been studied intensively in experiment and theory. They are a prototype for strongly correlated systems. Especially for bosons in a flat band, several interesting questions arise: What is the nature of the ground state? Are there regions in phase space where one can see a Bose transition?

The Bose-Hubbard model is used to visualize low energies on two-dimensional lattices which exhibit a lowest flat energy band. Up to the critical lattice filling constant, an eigenstate of the aforementioned band can be constructed by means of the charge density wave (CDW) as many-body ground state. Huber and Altman [1] explored ground states in the vicinity of the critical filling on the kagome lattice via a mean-field calculation; however, by restricting the calculation to a weakly interacting Hamiltonian.

The purpose of this talk is, firstly, to present similar results which are obtained by transferring their methods to the checkerboard lattice and, secondly, to demonstrate initial steps to extend to strong interactions. In this regard, one boson is added to the well-known ground state. The distribution of this additional particle seems to be localized, in contrast to the weakly interacting limit; here we observe a Bose condensation.

[1] S. Huber and E. Altman, PRB 82, 184502 (2010)

TT 69.3 Wed 15:30 A 053

Many-Body Anderson Localization of BECs in the Bose-Hubbard Model — •Roman Katzer[1], Cord Müller[2], and Johann Kroha[1] — [1]Universität Bonn — [2]Université de Nice, France

We have developed the transport theory for a Bose gas in the disordered Bose-Hubbard model in the regime of strong interactions, i.e. in the vicinity of the Mott lobes of vanishing Bose-Einstein condensate (BEC) amplitude. In contrast to previous approaches, we consider the Bose glass *not* as a state with vanishing averaged BEC amplitude with finite compressibility, but as the phase with *finite* average BEC amplitude but vanishing superfluid transport due to many-body Anderson localization of the interacting BEC wave functions and their many-body excitations. The theory is based on a calculation of the local many-body ground and excited states within a stochastic mean-field theory, treating the on-site Hubbard interaction exactly by diagonalizing the local part of the Bose-Hubbard Hamitonian in Fock space. Non-local effects of the interaction are neglected, analogous to Dynamical Mean-Field Theory. The transport theory for these hopping many-body states, including quantum interference processes ("Cooperons") is formulated as a generalization of the self-consistent theory of Anderson localization. The theory describes semiquantitatively the Mott localized phase ("Mott lobes"), the superfluid phase and the Bose glass phase as well as the respective phase transitions. In particular, the theory obeys the theorem of inclusions which states that in a disordered system there is no direct transition from the Mott phase to the superfluid phase.

TT 69.4 Wed 15:45 A 053

Thermalization of a Quenched Bose-Josephson Junction. —

•Anna Posazhennikova[1], Mauricio Trujillo-Martinez[2], and Johann Kroha[2] — [1]Royal Holloway University of London, UK — [2]Universitaet Bonn, Germany

The experimental realization and control of quantum systems isolated from the environment, in ultracold atomic gases relaunched the interest in the fundamental non-equilibrium problem of how a finite system approaches thermal equilibrium. Despite intensive research there is still no conclusive answer to this question. We investigate theoretically how a quenched Bose-Josephson junction, where the Josephson coupling is switched on instantaneously, approaches its stationary state. We use the field theoretical approach for bosons out of equilibrium in a trap with discrete levels, developed by us previously [1,2]. In this approach the operators for Bose-Einstein condensate (BEC) particles are treated on mean-field level, while excitations of the Bose gas in higher trap levels are treated fully quantum-mechanically. This leads to coupled equations of motion for the BEC amplitudes (Gross-Pitaevskii equation) and the quasiparticle propagators. The inelastic quasiparticle collisions responsible for the system relaxation during the time-dependent evolution are described within self-consistent second-order approximation.

[1] M. Trujillo-Martinez, A. Posazhennikova, J. Kroha, Phys. Rev. Lett. 103, 105302 (2009).
[2] M. Trujillo-Martinez, A. Posazhennikova, J. Kroha, New J. Phys. in press; arXiv:1406.5536v2.

TT 69.5 Wed 16:00 A 053

Non-Equilibrium Expansion Dynamics in the 2D Bose-Hubbard Model — Mauricio Trujillo-Martinez[1], •Anna Posazhennikova[2], and Johann Kroha[1] — [1]Universität Bonn — [2]Royal Holloway University of London, UK

We study the temporal expansion of an ultracold Bose gas in the 2D Bose-Hubbard model, where initially all bosons are put in one central site of the lattice. The time evolution of interacting many-body systems in more than one dimension has been a challenge for numerically exact methods. We therefore use the recently developed semi-analytical method for time evolution of Bose systems [1] where the many-body Hamiltonian is represented in an appropriate, local eigenbasis and the corresponding field operators are separated into classical (BEC) and quantum mechanical parts. As consequence, the classical Gross-Pitaevskii BEC dynamics is coupled to the quantum fluctuations. After a quench, i.e. after a sudden switch of the lattice nearest neighbor hopping, the bosons spead over the lattice in a nontrivial way. The low-density part at the rim of the bosonic cloud spreads ballistically, while the spread of the high-density part in the center of the cloud is inhibited by interaction-induced self-trapping effects, characteristic for lattice dynamics. As a result, the bosonic cloud separates spatially into a ballisic fore-runner and a nearly self-trapped central part. The expansion velocity of the fore-runner is consistent with the Lieb-Robinson limit.

[1] M. Trujillo-Martinez, A. Posazhennikova, J. Kroha, Phys. Rev. Lett. 103, 105302 (2009); New J. Phys. in press; arXiv:1406.5536v2.

TT 69.6 Wed 16:15 A 053

Relaxation of oscillations in a mass-imbalanced mixture of trapped ultracold Fermi gases — •Robert Bamler and Achim Rosch — University of Cologne, Germany

We present theoretical results on the center-of-mass oscillations of a mixture of two ultracold Fermi gases trapped in a harmonic potential. We investigate the dependency of the relaxation time on the mass difference and on the strength of the scattering between the two fermion species.

Ultracold atomic gases allow for the study of many-particle systems under highly controllable conditions. As interactions with the environment can be reduced to negligible amounts, these systems can be used to study the dynamics far from equilibrium and, in particular, the relaxation towards equilibrium due to collisions between the system's constituents.

We consider a mixture of two species of fermionic atoms in a harmonic trap. If both atom species have the same mass, then the center-of-mass oscillation of the atomic cloud around its equilibrium position is undamped even in the presence of interactions between the atoms. Moreover, Kohn's theorem states that the oscillation frequency is independent of the interaction strength. The situation changes if the two atomic species have slightly different masses. In this case, inter-species collisions lead to finite relaxation times for the two oscillatory modes and, with growing interaction strength, a merging of the two oscillatory modes. We study this transition quantitatively by investigating the memory matrix of the macroscopic coordinates.

TT 69.7 Wed 16:30 A 053

Directed motion of doublons and holes in periodically driven Mott insulators — •Maximilian Genske and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln, D-50937 Cologne, Germany

Periodically driven systems can lead to a directed motion of particles. We investigate this ratchet effect for a bosonic Mott insulator where both a staggered hopping and a staggered local potential vary periodically in time. If driving frequencies are smaller than the interaction strength and the density of excitations is small, one obtains effectively a one-particle quantum ratchet describing the motion of doubly occupied sites (doublons) and empty sites (holes). Such a simple quantum machine can be used to manipulate the excitations of the Mott insulator. For suitably chosen parameters, for example, holes and doublons move in opposite directions. To investigate whether the periodic driving can be used to move particles "uphill", i.e., against an external force, we study the influence of a linear potential $-gx$. For long times, transport is only possible when the driving frequency ω and the external force g are commensurate, $n_0 g = m_0 \omega$, with $\frac{n_0}{2}, m_0 \in \mathbb{Z}$. Ultimately, increasing the density of excitations leads to a breakdown of the one-particle picture. As an outlook, we thus discuss how interaction effects can be described by Floquet-Boltzmann equations.

TT 69.8 Wed 16:45 A 053

Tight binding models for ultracold atoms using maximally localized Wannier functions — •Julen Ibañez-Azpiroz[1], Asier Eiguren[2,3], Aitor Bergara[2,3], Giulio Pettini[4], and Michele Modugno[2,5] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Universidad del Pais Vasco, Bilbao, Spain — [3]Donostia International Physics Center, Spain — [4]Universita di Firenze and INFN, Italy — [5]Ikerbasque, Basque Foundation for Science, Spain

We discuss how to construct tight-binding models for weakly interacting ultracold atoms using maximally localized Wannier functions (MLWFs) [1]. The resulting models are shown to accurately describe the properties of the continuous systems with the use of few tunneling coefficients. First we work out a simple honeycomb lattice model directly related to the graphene physics [2]. Next we generalize the approach for including a vector potential and analyze a possible implementation of the Haldane model. We show that the commonly employed Peierls substitution does not yield a reasonable description of the effect of the vector potential on the tunneling coefficients [3], which in turn affects the topological phase diagram.

JIA acknowledges support from Helmholtz Gemeinschaft Deutscher-Young Investigators Group Program No. VH-NG- 717 (Functional Nanoscale Structure and Probe Simulation Laboratory).

[1] N. Marzari and D. Vanderbilt Phys. Rev. B 56, 12847 (1997)
[2] J. Ibañez-Azpiroz et al., Phys. Rev. A 87, 011602(R) (2013)
[3] J. Ibañez-Azpiroz et al., Phys. Rev. A 90, 033609 (2014)

15 min. break.

TT 69.9 Wed 17:15 A 053

Dimensional crossover and cold-atom realization of topological Mott insulators — Mathias S Scheurer[1], Stephan Rachel[2], and •Peter P Orth[1] — [1]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Institute for Theoretical Physics, TU Dresden, 01062 Dresden, Germany

Interacting cold-atomic gases in optical lattices offer an experimental approach to outstanding problems of many body physics. One important example is the interplay of interaction and topology which promises to generate a variety of exotic phases such as the fractionalized Chern insulator or the topological Mott insulator. Both theoretically understanding these states of matter and finding suitable systems that host them have proven to be challenging problems. Here we propose a cold-atom setup where Hubbard on-site interactions give rise to spin liquid-like phases: weak and strong topological Mott insulators. They represent the celebrated paradigm of an interacting and topological quantum state with fractionalized spinon excitations that inherit the topology of the non-interacting system. Our proposal shall help to pave the way for a controlled experimental investigation of this exotic

state of matter in optical lattices. Furthermore, it allows for the investigation of a dimensional crossover from a two- dimensional quantum spin Hall insulating phase to a three-dimensional strong topological insulator by tuning the hopping between the layers.

TT 69.10 Wed 17:30 A 053

Second order interaction corrections to the Fermi surface and the quasiparticle properties of dipolar fermions in three dimensions — •Jan Krieg, Philipp Lange, and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt, Germany

We have calculated the renormalized Fermi surface and the quasiparticle properties in the Fermi liquid phase of three-dimensional dipolar fermions to second order in the dipole-dipole interaction. Using parameters relevant to an ultracold gas of Erbium atoms, we have found that the second order corrections typically renormalize the Hartree-Fock results by less than one percent. On the other hand, if we use the second order correction to the compressibility to estimate the regime of stability of the system, the point of instability is already reached for a significantly smaller interaction strength than in the Hartree-Fock approximation.

TT 69.11 Wed 17:45 A 053

Artificial gauge fields in extra dimensions — •Julius Ruseckas[1], Gediminas Juzeliunas[1], Ian Spielman[2,3], Alessio Celi[4], Pietro Massignan[4], Nathan Goldman[5], and Maciej Lewenstein[4,6] — [1]Institute of Theoretical Physics and Astronomy, Vilnius University, A. Goštauto 12, Vilnius, LT-01108 Lithuania — [2]Joint Quantum Institute, University of Maryland, College Park, Maryland 20742-4111, USA — [3]National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA — [4]ICFO-Institut de Ciencies Fotoniques, Mediterranean Technology Park, E- 08860 Castelldefels (Barcelona), Spain — [5]Laboratoire Kastler Brossel, CNRS, UPMC, ENS, 24 rue Lhomond, F- 75005 Paris, France — [6]ICREA-Institucio Catalana de Recerca i Estudis Avancats, E-08010 Barcelona, Spain

We demonstrate [1] that one can engineer a two-dimensional lattice with nonzero synthetic magnetic flux using atoms in a standard one-dimensional optical lattice. The additional dimension appears due to laser-assisted transitions between the atomic sub-levels in the ground state manifold. A distinctive feature of the proposed scheme is the sharp boundaries in the extra dimension, a feature that is difficult to implement for the atoms in optical lattices in the real-space. The boundaries of the extra dimension can be closed down using additional laser-assisted transitions. which leads to a remarkably simple realisation of the fractional (Hofstadter butterfly-type) spectrum.

[1] A. Celi, P. Massignan, J. Ruseckas, N. Goldman, I. B. Spielman, G. Juzeliunas, and M. Lewenstein,
Phys. Rev. Lett. 112, 043001 (2014).

TT 69.12 Wed 18:00 A 053

Phase Space Interactions and Exchange Quasienergy — •Lingzhen Guo[1,2], Modan Liu[1,3], and Michael Marthaler[1] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, SE-41296 Göteborg, Sweden — [3]Department of Physics, Beijing Normal University, Beijing 100875, China

In this work, we investigate the dynamics of many interacting atoms trapped in a one dimensional (1D) harmonic potential and driven by laser beams. By going to a rotating frame, we transform the one dimensional (spatial)interaction potential to a two dimensional potential in phase space, which only depends on the phase space distance under rotating wave approximation (RWA). The *phase space interaction potentials*, describing the interaction between slow evolution modes of interacting particles under RWA, are created by exchanging their fast oscillating modes. We quantize the phase space interactions and apply it to the study of driven multistable systems. We propose the concept of *exchange quasienergy* and calculate it for the system of two driven half-spin fermions, which is the difference of quasienergies between the singlet and triplet states. In theory, our work provides a new mechanism of creating interactions by exchanging not intermediate bosons but the interacting particles themselves. In experiments, the novel effects related to exchange quasienergy can be directly measured and may bring a new way to manipulate entangled states of atoms.

TT 69.13 Wed 18:15 A 053

B-DMFT with strong-coupling solver for inhomogeneous systems — Anna Kauch[1], •Jaromir Panas[2], Dieter Vollhardt[3], and Krzysztof Byczuk[2] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 18221 Praha, Czech Republic — [2]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warszawa, Poland — [3]Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

We employ bosonic dynamical mean-field theory (B-DMFT) [1] with a strong-coupling impurity solver [2] to compute the particle density and condensate fraction of strongly interacting, inhomogeneous Bose systems. We apply the method to bosons in optical lattices with inhomogeneities due to the trapping potential and impurities. The influence of these inhomogeneities on the transition between the Mott insulating phase and the Bose-Einstein condensate is discussed.

[1] K. Byczuk and D. Vollhardt, Phys. Rev. B 77, 235106 (2008).
[2] A. Kauch, K. Byczuk, and D. Vollhardt,
Phys. Rev. B 85, 205115 (2012).

TT 69.14 Wed 18:30 A 053

Anderson and Mott transitions in the presence of spin-dependent disorder — •Jan Skoliomwski[1], Krzysztof Byczuk[1], and Dieter Vollhardt[2] — [1]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, ul. Pasteura 5, PL-02-093 Warszawa, Poland — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135, Augsburg, Germany

Recent experiments with ultra-cold atoms in optical lattices [1] have caused us to investigate the phase diagram of correlated lattice fermions in the presence of spin-dependent disorder [2,3]. To this end we solved the Anderson-Hubbard model with a spin-dependent random potential within the dynamical mean-field theory, using the geometrically averaged local density of states to make the theory sensitive to Anderson localization [4]. The paramagnetic ground state phase diagram was determined. Spin-dependent disorder is seen to destabilize the metallic solution, in contrast to the usual case of spin-independent disorder [5]. For strong disorder above the critical point for the Mott transition novel spin-dependent localized phases are found.

[1] D. McKay and B. DeMarco, New J. Phys. 12, 055013 (2010).
[2] K. Makuch et al., New J. Phys. 15, 045031 (2013).
[3] R. Nanguneri et al., Phys. Rev. B 85, 134506 (2012).
[4] V. Dobrosavljevic et al., Europhys. Lett. 62, 76 (2003).
[5] K. Byczuket al., Phys. Rev. Lett. 94, 056404 (2005).

TT 69.15 Wed 18:45 A 053

Dirac cones merging transition and geometric phase in Stuckelberg interferometer with cold atoms — •Lih-King Lim — MPI PKS, Dresden, Germany — Institut d'Optique, Palaiseau, France

Dirac cones in the energy spectrum lies at the heart of many interests in studying two-dimensional crystals such as graphene or MoS_2. Besides its unusual density-of-states, a Dirac cone possesses geometric information hidden in the wavefunction, e.g., Berry phase and mass. The latter determines the type of topological state of matter. Thanks to recent progresses in engineering two-dimensional topological band structure with cold atoms, we study a Stuckelberg interferometer realized via Bloch-oscillations-type experiment. The paths that bring Bloch waves to interfere are made of the two energy levels in between a pair of Dirac cones. We show that the interference pattern contains an extra phase shift that has a geometric origin, in the form of an open path Berry phase of the wavefunction. It is revealed in the final inter-band transition probability and hence, it is a gauge invariant quantity. This phase can serve as a robust bulk probe for topological band structures realized with artificial crystals.

[1] L.-K. Lim, J.N. Fuchs, G. Montambaux,
Phys. Rev. Lett. 112, 155302 (2014).

TT 70: Correlated Electrons: Spin Systems and Itinerant Magnets – Chiral Magnets (jointly with MA)

Time: Wednesday 18:00–19:15 Location: H 3005

TT 70.1 Wed 18:00 H 3005

Gracing incidence small angle neutron scattering of incommensurate magnetic structures in MnSi thin films — Birgit Wiedemann[1], Shilei Zhang[2], Yury Khaydukov[3,4], Thorsten Hesjedal[2], Olaf Soltwedel[3,4], Thomas Keller[3,4], Sebastian Mühlbauer[5], •Alfonso Chacon[1,5], Christian Pfleiderer[1], and Peter Böni[1] — [1]Physik Department, Technische Universität München, Germany — [2]Clarendon Laboratory, Department of Physics, University of Oxford, UK — [3]Max-Planck-Institut für Festkörperforschung, Germany — [4]Max Planck Society, Outstation at FRM-II, Germany — [5]Forschungsneutronenquelle Heinz Maier Leibnitz, Technische Universität München, Germany

The topological stability of skyrmions in bulk samples of MnSi and the observation of spin transfer torque effects at ultra-low current densities have generated great interest in skyrmions in chiral magnets as a new route towards next generation spintronics devices. Yet, the formation of skyrmions in MBE grown thin films of MnSi reported in the literature is highly controversial. We report gracing incidence small angle neutron scattering (GISANS) of the magnetic order in selected thin films of MnSi grown by state of the art MBE techniques. In combination with polarised neutron reflectometry (PNR) and magnetisation measurements of the same samples our data provide direct reciprocal space information of the incommensurate magnetic order, clarifying the nature of magnetic phase diagram.

TT 70.2 Wed 18:15 H 3005

Neutron spin-echo spectroscopy of spin fluctuations in the skyrmion lattice phase of MnSi — •Franz Haslbeck[1], Jonas Kindervater[1], Andreas Bauer[1], Wolfgang Häussler[1,2], Peter Böni[1], and Christian Pfleiderer[1] — [1]Physik-Department, Technische Universität München, Germany — [2]Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany

Recent theoretical studies suggest that the skyrmion lattice phase in chiral magnets such as MnSi is stabilised by thermal spin fluctuations [1,2]. We report an experimental study of the quasielastic spectrum of spin fluctuations in the skyrmion lattice phase of MnSi. Using the so called MIEZE spin-echo technique at the spectrometer RESEDA at FRM II we achieved an unprecedented resolution below 1 μeV going well beyond a first preliminary study [3]. Applying a magnetic field parallel and perpendicular to the neutron beam allowed us to study the fluctuations in and out of plane of the skyrmion lattice.

[1] S. Mühlbauer *et al.*, Science **323**, 915 (2009).
[2] S. Buhrandt, L. Fritz, Phys. Rev. B **88**, 195137 (2013).
[3] R. Georgii *et al.*, Appl. Phys. Lett. **98**, 073505 (2011).

TT 70.3 Wed 18:30 H 3005

NMR-on site-probe of field-modulated and Skyrmion states in chiral magnets: FeGe and Cu_2OSeO_3 — •Michael Baenitz, Mayukh Majumder, Panchanan Khuntia, Hiroshi Yasuoka, and Markus Schmidt — MPI for the Chemical Physics of Solids, 01187 Dresden, Germany

Cubic FeGe is a prototype B20 chiral magnet (with $T_c = 280$K) which allows to study chiral excitations directly "on-site" via the ^{57}Fe nucleus because of its S=1/2 nuclear spin. NMR provides the local susceptibility (hyperfine field), the dynamic susceptibility (spin lattice relaxation rate SLRR = $1/T_1$) and the spin-spin interaction (spin-spin relaxation rate SSRR = $1/T_2$). Measurements were performed on crushed single crystals of ^{57}Fe enriched FeGe material between 2-300 K in zero and applied magnetic fields. Helical- conical- and field-polarized- states could be clearly identified from NMR and critical dynamics at these transitions are investigated. The field dependence of H_{hf}, SLRR and SSRR was studied in great detail at various temperatures below T_c. Especially an evidence of the Skyrmion -A- phase formation is given by NMR. Cubic Cu_2OSeO_3 is an oxide with a ferrimagnetic transition at about 60 K. Its magnetic phase diagram - including the Skyrmion phase - is very similar to FeGe. We present first ^{63,65}Cu NMR results on single crystals at zero field and in modulation fields.

TT 70.4 Wed 18:45 H 3005

Spin chirality flip in $Fe_{1-x}Co_xSi$ — •Sven-Arne Siegfried[1], Evgeny.V. Altenbayev[2,3], Nadezhda M. Chubova[2,3], Vadim Dyadkin[4,2], Dirk Menzel[5], Charles D. Dewhurst[6], André Heinemann[1], Dimitry Chernyshov[4], Ravil A. Sadykov[7,8], Sergey N. Axenov[7], Ludmila N. Formicheva[8], Anatoly V. Tsvyashchenko[8], Andreas Schreyer[1], and Sergey V. Grigoriev[2,3] — [1]Helmholtz-Zentrum Geesthacht, Germany. — [2]Petersburg Nuclear Physics Institute, Russia. — [3]Saint- Petersburg State University, Russia. — [4]SwissNorwegian Beamlines at ESRF, France. — [5]TU Braunschweig, Braunschweig, Germany. — [6]Institute Laue-Langevin, France. — [7]Institute for Nuclear Research, Russia. — [8]Institute for High Pressure Physics,Russia.

Recently the experimental evidence was given for the flip of the spin helix chirality in the two Fe-based germanide compounds $Mn_{1-x}Fe_xGe$ [1] and $Fe_{1-x}Co_xGe$ [2]. In this talk we report the similar effect for the Fe-based silicide $Fe_{1-x}Co_xSi$ at a critical concentration x_c. We have synthesized single-crystalline $Fe_{1-x}Co_xSi$ compounds with x running from 0.5 to 0.7 via Czochralski-method. SQUID magnetization measurements have shown the magnetic ordering of all these samples below T_c. At the critical concentration $x_c \approx 0.65$ we observed a transformation of the helical structure to a ferromagnetic one ($|\mathbf{k}_s| \to 0$). Polarized small-angle neutron scattering revealed the different sign of the spin helicity for compounds with $x > x_c$ and $x < x_c$.

[1] S.V. Grigoriev et al.,PRL. 110, 207201 (2013).
[2] S.V. Grigoriev et al.,PRB 90, 174414 (2014).

TT 70.5 Wed 19:00 H 3005

$BaMn_9[VO_4]_6(OH)_2$, a novel candidate for the observation of a Skyrmion lattice — •Angela Möller[1], Kewen Sun[1], Vladimir Gnezdilov[2,3], and Peter Lemmens[3] — [1]Department of Chemistry and TcSUH, University of Houston, United States — [2]ILTPE NAS, Kharkov, Ukraine — [3]IPKM, TU-BS, Braunschweig, Germany

The search for topologically stable vortex-like objects (Skyrmions) in insulating chiral magnets lead to their discovery in Cu_2OSeO_3 [1]. We will show that the combination of certain structural features, such as chirality and frustration might expedite the finding of new candidates of this rare class. A chiral paddle-wheel type of structure featuring geometric frustration has been reported for the metrically cubic title compound with ferrimagnetic, Tc=18 K, and dielectric anomalies [2]. Interestingly, Raman scattering shows magnetoelastic coupling of several phonons but no spontaneous symmetry reduction. This is considered a prerequisite for the existence of a Skyrmion lattice.

This work was supported by the NSF (DMR-1149899) and RTG-DFG 1953/1.

[1] Seki et al., Science 336, 198 (2012);
T. Adams et al., PRL 108, 237204 (2012).
[2] K. Sun et al., Inorg. Chem. dx.doi.org/10.1021/ic502266k.

TT 71: Correlated Electrons: Poster Session

Time: Wednesday 15:00–18:00 Location: Poster B

TT 71.1 Wed 15:00 Poster B

Surface properties of SmB_6 from x-ray photoemission spectroscopy — •Nadine Heming[1], Uwe Treske[1], Martin Knupfer[1], Bernd Büchner[1,2], Dmytro Inosov[2], Natalya Y. Shitsevalova[3], Volodymyr B. Filipov[3], Stephan Kraus[4], and Andreas Koitzsch[1] — [1]Institute for Solid State Research, IFW Dresden — [2]Institut für Festkörperphysik, TU Dresden — [3]Institute for Problems of Material Sciences, Kiev — [4]BESSY II, Berlin

The mixed valence compound SmB_6 has been well known for its anomalous low temperature resistivity behavior for decades: At temperatures below 50 K, SmB_6 transmutes from a metal to an insulator but shows residual resistivity for temperatures less than 5K. Renewed interest in this material comes from theoretical proposals, predicting topological protected surface states making this compound the prime candidate for the new material class of '"Topological Kondo Insulators'". Indeed, elaborate transport experiments have evidenced that the residual conductivity occurs only at the surface. However, it is generally well known that the surface of f-systems undergoes valence changes and reconstructions, which may also influence the surface properties of this material. Applying surface sensitive soft x-ray photoemission spectroscopy, we have investigated the surface properties of freshly cleaved SmB_6 single crystals at 15K monitoring the Sm valance, the chemical state of boron as well as the surface stoichiometry, and also the development of these over time and with increased temperature: We have found that the surface shows an unexpected complexity stemming from both intrinsic and extrinsic changes.

TT 71.2 Wed 15:00 Poster B

Hidden order symmetry and superconductivity in Heavy Fermions investigated by quasiparticle interference — •Alireza Akbari[1,2] and Peter Thalmeier[3] — [1]Asia Pacific Center for Theoretical Physics, POSTECH, Pohang, Gyeongbuk 790-784, Korea — [2]MPI for Solid State Research, Stuttgart, Germany — [3]MPI for the Chemical Physics of Solids, Dresden, Germany

The hidden order (HO) in URu_2Si_2 has been determined as a high rank multipole formed by itinerant 5f-electrons with distinct orbital structure imposed by the crystalline electric field. Because this can lead to a considerable number of different multipoles it is of great importance to use microscopic techniques that are sensitive to their subtle physical differences. Here we investigate whether quasiparticle interference (QPI) method can distinguish between the two most frequently proposed HO parameter models: the even rank-4 hexadecapole and the odd-rank-5 dotriacontapole model. We obtain the quasiparticle dispersion and reconstructed Fermi surface in each HO phase adapting an effective two-orbital model of 5f bands that reproduces the main Fermi surface sheets of the para phase. We show that the resulting QPI spectrum reflects directly the effect of fourfold symmetry breaking in the rank-5 model which is absent in the rank-4 model. Therefore we suggest that QPI method should give a possibility of direct discrimination between the two most investigated models of HO in URu_2Si_2. Furthermore the signature of proposed chiral d-wave superconducting (SC) order parameter in QPI of the coexisting HO+SC phase is investigated.

TT 71.3 Wed 15:00 Poster B

Site dependence of the Kondo scale in $CePd_{1-x}Rh_x$ evidenced by thermopower — •Ulrike Stockert[1], Stefanie Hartmann[1], Micha Deppe[1], Nubia Caroca-Canales[1], Christoph Geibel[1], Julian Sereni[2], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden — [2]Division Bajas Temperaturas, Centro Atómico Bariloche, Argentina

$CePd_{1-x}Rh_x$ undergoes a continuous evolution from ferromagnetic order in CePd to an intermediate-valence (IV) ground state for CeRh. Close to the disappearance of magnetic order at $x_{cr} \approx 0.87$ unusual behavior of the ac susceptibility and the specific heat was observed. It was explained with a broad distribution of local Kondo temperatures T_K from below 2 K to above 50 K due to the disorder introduced by Pd-Rh exchange.

The thermopower S is very sensitive to Kondo scattering even for diluted 4f systems. In Ce compounds a large positive maximum in $S(T)$ is usually observed around T_K. We studied $S(T)$ in $CePd_{1-x}Rh_x$ in order to evaluate the presence of Kondo scattering and the involved enery scales. Pure CeRh shows typical IV behavior with a large maximum at 220 K and small values at low T. Already 5 % Pd substitution leads to a strong enhancement of the low-T thermopower. Even larger values are found around x_{cr}, while the high-T maximum shifts only moderately. Our results are in line with the existence of low (local) Kondo scales in the presence of IV behavior at high Rh content $x > x_{cr}$. For lower Rh content a decreasing (average) Kondo scale is found.

TT 71.4 Wed 15:00 Poster B

Electron Spin Resonance of the itinerant ferromagnets $CeCrGe_3$ and $LaCrGe_3$ — •Jörg Sichelschmidt[1], Thomas Gruner[1], Christoph Geibel[1], Debarchan Das[2], and Zakir Hossain[2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden — [2]Department of Physics, Indian Institute of Technology, Kanpur 208016, India

We report Electron Spin Resonance (ESR) of the itinerant ferromagnets $CeCrGe_3$ and $LaCrGe_3$. Both compounds show well defined and very similar spectra of itinerant Cr 3d spins in the paramagnetic temperature region, adding another two examples of a rarely observed conduction electron spin resonance in 3d metals.

Upon cooling and crossing the Cr-FM ordering (below around 90 K) strong spectral structures start to dominate the resonance spectra in a quite different manner in $CeCrGe_3$ and $LaCrGe_3$. In the Ce-compound the resonance is visible in the paramagnetic region only whereas in the La-compound the resonance can be followed far below the FM ordering temperature. This behavior will be discussed in terms of the specific interplay between Ce and Cr magnetism which appears quite remarkable since $CeCrGe_3$ displays Kondo lattice behavior with a heavy fermion specific heat even in the magnetically ordered state [1].

[1] D. Das, T. Gruner, H. Pfau, U. B. Paramanik, U. Burkhardt, C. Geibel, and Z. Hossain, J. Phys. Condens. Matter 26, 106001 (2014).

TT 71.5 Wed 15:00 Poster B

de Haas-van Alphen oscillations in (La,Ce)$TiGe_3$ — •J. Grasemann[1,2], M. Uhlarz[1], W. Kittler[3], V. Fritsch[3,4], O. Stockert[5], T. Förster[1], J. Wosnitza[1,2], and H. v. Löhneysen[3] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]TU Dresden, 01062 Dresden, Germany — [3]Karlsruhe Institute of Technology, 76049 Karlsruhe, Germany — [4]Institut für Physik, Universität Augsburg, 86135 Augsburg — [5]Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany

$CeTiGe_3$ is one of the few Kondo-lattice compounds which order ferromagnetically ($T_C \approx 14$ K); $LaTiGe_3$ may be used as its nonmagnetic reference, since both compounds crystallize in the same hexagonal perovskite structure [1, 2]. We report on angular-resolved de Haas-van Alphen oscillations in single crystals of $CeTiGe_3$, $LaTiGe_3$, and $Ce_{0.1}La_{0.9}TiGe_3$ grown from Ge flux, measured in magnetic fields up to 13 T in a cantilever-type torque magnetometer. We found several dHvA frequencies, ranging in $CeTiGe_3$ from 100 to 530 T and with effective masses around $0.7\,m_0$, featuring a comparably weak angular dependence. Further, we give an interpretation of our results on the basis of DFT calculations of the electronic band structure of $CeTiGe_3$ and $LaTiGe_3$.

[1] P. Manfrinetti et al., Solid State Commun. **135** (2005) 444-448.
[2] W. Kittler et al., Phys. Rev. B **88** (2013) 165123

TT 71.6 Wed 15:00 Poster B

DFT Study on (La,Ce)$TiGe_3$ — •Tobias Förster[1], Helge Rosner[2], Jacob Grasemann[1], Marc Uhlarz[1], Wolfram Kittler[3], Veronika Fritsch[3,4], Oliver Stockert[2], Jochen Wosnitza[1], and Hilbert v. Löhneysen[3] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [3]Karlsruher Institut für Technologie, 76049 Karlsruhe, Germany — [4]Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

$CeTiGe_3$ presents the rare case of a ferromagnetically ($T_C \approx 14$ K) ordered Kondo-lattice compound and is probably the first known example of an intermetallic hexagonal perovskite of the $BaNiO_3$ structure type. $LaTiGe_3$ is the nonmagnetic analogue. To clarify the interplay

between structural, localized, and itinerant degrees of freedom an accurate knowledge of the electronic band structure is necessary. Here, we present detailed comparative electronic structure calculations for both compounds. Applying full potential density functional calculations in different approximations, we attempt to separate the influence of different parameters of the crystal structure on the topology and character of the respective Fermi surfaces. We compare our calculated results with de Haas-van Alphen measurements.

TT 71.7 Wed 15:00 Poster B

Heavy fermion behaviour in the high pressure structure of $CeSb_2$ — •Vitaly Fedoseev[1], Zhuo Feng[1], Yang Zou[1], Terence Giles[2], Philipp Niklowitz[2], Heribert Wilhelm[3], Giulio Lampronti[4], and F. Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — [2]Department of Physics, Royal Holloway, University of London, Egham TW20 0EX, UK — [3]Beamline I15, Diamond Light Source, Didcot OX11 0DE — [4]Department of Earth Sciences, University of Cambridge, Cambridge CB2 3EQ, UK

The Kondo lattice system $CeSb_2$ crystallises in the orthorhombic $SmSb_2$ structure and exhibits a series of magnetic phase transitions at low temperature. It has been reported to become ferromagnetic below 15 K, with the ordered moment oriented within the basal plane, and to undergo two further transitions at 9K and 12K [1]. These transition are suppressed above a hydrostatic pressure $p_c \simeq 16$ kbar. We present high pressure transport and x-ray diffraction results, which examine the high pressure state of $CeSb_2$. Our findings suggest that $CeSb_2$ undergoes a drastic structural change at p_c into a new and now fully resolved crystal structure. Whereas in the low pressure structure, $CeSb_2$ is a local moment magnet, in the high pressure structure it exhibits transport properties characteristic of a heavy fermion material with a low Kondo temperature scale of the order of 10 K.

[1] Bud'ko et al. PRB **57**, 21 (1998)

TT 71.8 Wed 15:00 Poster B

Crystal field splitting in $CePt_5$: magnetic analysis and Raman spectroscopy — •Martin Zinner[1], Benedikt Halbig[2], Utz Bass[2], Christian Praetorius[1], Jean Geurts[2], and Kai Fauth[1] — [1]Universität Würzburg, Experimentelle Physik II, 97074 Würzburg, Germany — [2]Universität Würzburg, Experimentelle Physik III, 97074 Würzburg, Germany

The crystal electric field (CF) is an essential factor determining the paramagnetic response of rare earth ions in solids. In Ce intermetallics, Kondo screening can additionally modify the magnetic behavior and it may then prove difficult to disentangle the two. In the hexagonal surface intermetallic $CePt_5$, grown on Pt(111) [1], we find two distinct sets of CF parameters which both account rather well for the anisotropic magnetic susceptibility and its temperature dependence. Different strengths of Kondo screening have to be assumed in the two cases in order to obtain quantitative agreement with experimental results.

Discriminating between the two solutions requires an independent determination of the CF splitting. We shall report on our attempts to obtain this information from electronic Raman scattering. Raman signal is indeed even obtained from $CePt_5$ specimens with a thickness of just two unit cells. We shall discuss the identification of electronic Raman losses by comparison with $LaPt_5$ as well as the dependence of the Raman features on temperature and thickness of the intermetallic film.

[1] J. Kemmer, C. Praetorius *etal.*, Phys. Rev. B **90**, 195401 (2014).

TT 71.9 Wed 15:00 Poster B

Electronic and magnetic structure of $RENi_2Mn_x$-compounds (RE = rare earth, x = 0, 0.25, 0.5, 0.75, 1, 1.25) with respect to $ErNi_2Mn_x$ — •Kamil Balinski[1], Artur Chrobak[3], T.V. Kuznetzsova[2], N.V. Mushnikov[2], V.V. Marchenkov[2], and Karsten Küpper[1] — [1]Department of Physics, Osnabrück University, Germany — [2]Institute of Metal Physics, 620990 Ekaterinburg, Russia — [3]Department of Physics, University of Silesia in Katowice, Poland

Rare earth (RE) and transition metal (T) compounds are research field since the 1960s. Because of huge magnetocalorical effect and giant magnetostriction the RE-T-compounds are excellent for applications like magnetic cooling or hydrogen storage devices. Besides of that RE-Ni_2-type of alloys are, due to the relatively simple crystal structure and the fact that Ni_2 does not indicate any magnetic moment, excellent candidates for studies of magnetic behavior of RE's and their binding partners. The electronic structure of $ErNi_2Mn_x$ (x = 0, 0.25, 0.5, 0.75, 1, 1.25) is characterized by XPS and ResPES, the magnetic structure is investigated by SQUID and PPMS techniques, and resistivity measurements are made. Variation in Mn concentration revealed the position of Mn 3d-states at 1.7 eV. The XPS intensity at 1.7 eV can be correlated with the behavior of the Curie temperature and the resistivity. While similar $RENi_2Mn_x$-systems, where RE had been replaced by Gd and Tb, highest resistivity, Curie temperature and the highest Mn 3d-valence band state intensity were observed at x = 0.5. $ErNi_2Mn_x$-system behave different and show the mentioned maxima at x = 1.25.

TT 71.10 Wed 15:00 Poster B

Multi-impurity Anderson models: geometry and entanglement — •Benjamin Mille, Tizian Müller, and Ralf Bulla — Institut für Theoretische Physik, Universität zu Köln

Block-tridiagonalisation methods allow to map multi-impurity Anderson models in arbitrary geometry and dimension onto models of M coupled chains (M = number of impurities). The resulting chain model can then be used as a starting point for renormalization group and iterative methods. Here we discuss how to combine the logarithmic discretization - an essential feature of Wilson's Numerical Renormalization Group - with the general tridiagonalisation scheme. This corresponds to the mapping of the original model onto a Wilson ladder, the generalization of the Wilson chain obtained for the single-impurity case. Furthermore we investigate - via exact diagonalization of small clusters - how the entanglement between two spatially separated Anderson impurities falls off with their distance.

TT 71.11 Wed 15:00 Poster B

Nonequilibrium dynamics of the pseudo gap single impurity Anderson model — •Julian Musshoff[1], Christian Kleine[2], and Frithjof B. Anders[2] — [1]Forschungszentrum Jülich GmbH, Institute for Advanced Simulation, 52425 Jülich, Germany — [2]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

In the single impurity Anderson model with a pseudo-gap density of states, modeled by a power law $\rho(\epsilon) \propto |\epsilon|^r$, a local moment phase and a strong coupling phase are separated by a quantum critical point (QCP). We investigate the real-time dependence of the double occupancy of the impurity due to quenches in one phase and over the QCP using the time-dependent numerical renormalization group (TD-NRG). We show that the double occupancy equilibrates to a steady state for long times. We present a time-dependent perturbation theory which becomes exact at short times. The short-time evolution of our TD-NRG data excellently agrees with this perturbation theory providing an analytical expression of the relevant time scales for the short-time dynamics. We are able to trace back the differences between the results obtained by a time-dependent Gutzwiller variational approach and by the TD-NRG to the wave-function ansatz in the Gutzwiller approach.

TT 71.12 Wed 15:00 Poster B

Cobalt adatoms on Graphene: role of the realistic interaction matrix in a QMC simulation — •Igor Krivenko[1], Maria Valentyuk[1], Ersoy Sasioglu[2], Priyanka Seth[3], Michel Ferrero[3], Olivier Parcollet[4], and Alexander Lichtenstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich — [3]Centre de Physique Théorique, École Polytechnique, France — [4]Institut de Physique Théorique, CEA-Saclay, France

We have theoretically studied the local spectra and magnetic properties of the cobalt impurities on the graphene at the low temperatures. In our studies we have employed the DFT++ method in the projector augmented wave (PAW) basis set using the VASP code, and a new hybridization expansion CT-QMC solver from the TRIQS project (Toolbox for Research on Interacting Quantum Systems). We have been interested in the observation of the spin and orbital Kondo effect in the different adatom geometries (hollow-position/top-position). Another question of the interest has been to study the effect of different approximations for the local interaction matrix on the impurity spectrum. In order to reproduce the multiplet structure of the cobalt d-shell, one has to consider interactions beyond a simple density-density approximation. With our new hybridization expansion solver we have been able to treat a U-matrix, parametrized by 3 Slater integrals (129 non-vanishing matrix elements) and a realistic U-matrix, obtained by

means of the Constrained RPA method (157 elements).

TT 71.13 Wed 15:00 Poster B

Multi-spin multi-channel Kondo box problem — •Mirek Hänsel, Andrej Schwabe, and Michael Potthoff — Institut für Theoretische Physik, Universität Hamburg

In a quantum box, where one or several quantum spins are coupled by a weak antiferromagnetic local exchange J to a system of non-interacting conduction electrons, the standard Kondo effect is cut by the finite system size. The residual finite-size Kondo effect can be described by perturbation theory in J. We show that the effective low-energy physics is given by a central-spin model where typically each impurity spin couples to the spin of a completely delocalized conduction-electron eigenstate at the Fermi edge. Different screening channels are given for the case of orthogonal eigenstates. We discuss the general case of several spins and several channels by analyzing various geometries, e.g., one-dimensional chains and two-dimensional lattices with different boundary conditions, and different geometrical setups of the impurity spins. The couplings in the effective central-spin model and the resulting magnetic structure are calculated as functions of the conduction-electron density and the geometry.

TT 71.14 Wed 15:00 Poster B

Towards a Matrix Product State based description of steady-state non-equilibrium physics in 1D correlated quantum systems using Lindblad driving — •Frauke Schwarz[1], Ireneusz Weymann[2], Jan von Delft[1], and Andreas Weichselbaum[1] — [1]Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, Munich, Germany — [2]Faculty of Physics, Adam Mickiewicz University, Poznań, Poland

The Kondo effect in quantum impurity models in equilibrium is well-understood by means of the Numerical Renormalization Group (NRG). To extend the description of Kondo physics to situations of steady state non-equilibrium, we want to combine the ideas of NRG with the Lindblad approach to open quantum systems. For this purpose, we introduce additional reservoirs described by Lindblad terms in the Liouville equation which restore the continuum properties of the discretized leads that are coupled to the impurity. This enables us to define the temperature and the chemical potential for each lead independently. To reduce the dimensionality of the problem we employ the stochastic quantum trajectory approach to solve the underlying Lindblad equation.

Several ideas on how to define adequate Lindblad operators will be presented together with their implications for the calculation of the quantum trajectories based on Matrix Product States.

TT 71.15 Wed 15:00 Poster B

Temperature dependent properties in the infinite-dimensional Hubbard model with a magnetic field — •Markus Dutschke[1], Liviu Chioncel[1,2], and Junya Otsuki[3] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [3]Department of Physics, Tohoku University, Sendai 980-8578, Japan

We investigate the temperature and field dependence of the spectral function, the effective mass enhancement and the magnetisation of the infinite-dimensional Hubbard model in a magnetic field. We compare results for different interaction strengths at half-filling, near half-filling and quarter-filling. These are achieved by using dynamical mean-field theory (DMFT) with a continuous-time quantum monte carlo (CT-QMC) impurity solver and are compared with some NRG results.

TT 71.16 Wed 15:00 Poster B

Influence of strong disorder on incoherent transport near the Mott transition: Statistical DMFT approach — •Milos Radonjic[1,2], Darko Tanaskovic[2], and Vladimir Dobrosavljevic[3] — [1]Center for Electronic Correlations and Magnetism, Theoretical Physics III, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — [3]Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA

We present the study of disordered half-filled Hubbard model within the Statistical dynamical mean field theory, which is a unique theoretical method reliable and controllable in a wide temperature, disorder and interaction range. We have successfully applied this method, for the first time, on the finite size cubic lattice, at finite temperature.

The results show that the finite size effects are negligible already on the lattice with 6*6*6 sites (except at the lowest temperatures, deep in the Fermi liquid regime). Also we confirmed that disorder is strongly screened on the metallic side of the Mott MIT and that inelastic scattering is dominant outside of the Fermi liquid region. We defined a local resistivity and proposed a resistor network method for calculating lattice dc resistivity. Two types of sites can be identified: strongly correlated - with the local occupation close to 1, and weakly correlated - away from local half-filling. Strongly correlated sites are responsible for strong, non-monotonic temperature dependence of the resistivity.

TT 71.17 Wed 15:00 Poster B

Electronic correlations and spin-orbit coupling in d^4 osmates — •Vladislav Pokorný[1] and Jan Kuneš[2] — [1]Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

We employ the combination of the density functional theory and the dynamical mean-field theory to investigate the electronic correlations in heavy transition metal compounds with partially filled t_{2g} levels such as d^4 osmates which were prepared recently. Using the hybridization-expansion, continuous-time quantum Monte Carlo impurity solver we study the combined influence of electron correlations and spin-orbit coupling effects on the the electronic and magnetic structure of these systems.

TT 71.18 Wed 15:00 Poster B

NMR on the quantum critical ferromagnet $YbNi_4P_2$: Evidence for a large basal plane local anisotropy — •Rajib Sarkar[1], Marco Günter[1], Cornelius Krellner[3], Michael Baenitz[2], Christoph Geibel[2], and Hans-Henning Klauss[1] — [1]IFP, TU Dresden, D-01069 Dresden, Germany — [2]MPI-CPFS, D-01187 Dresden, Germany — [3]Goethe University Frankfurt, D-60438 Frankfurt am Main, Germany

In the last 10 years there was growing evidence both from theoretical work and experimental observations that a ferromagnetic (FM) quantum critical point (QCP) cannot exist in a pure system, because the transition becomes first order before reaching the QCP. Therefore the recent report of clear evidence for a FM-QCP in the heavy fermion compound $YbNi_4P_2$ attracted considerable attention. While the Bravais lattice of this compound is tetragonal, resulting in isotropic in-plane macroscopic magnetic properties, the local symmetry on the Yb site (and on the P-site) is lower, orthorhombic. Therefore some in-plane anisotropy of local magnetic properties is expected, which could however not yet been studied because of the absence of related effects on macroscopic properties. We performed ^{31}P NMR investigations on a grain aligned polycrystalline sample of $YbNi_4P_2$. We observed three structures in the NMR spectra, which present quite different T-dependence of the respective Knight shifts. An analysis of these results provides a clear evidence for strong local in-plane anisotropy of the Yb-moment due to the orthorhombic crystal electric field. Implication for the magnetic ordered state shall be discussed.

TT 71.19 Wed 15:00 Poster B

Single crystal growth of the heavy fermion compounds $YbRh_2Si_2$ and $YbNi_4P_2$ — •Constantin Butzke, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany

Heavy fermion systems are model systems to unravel the exciting physics around quantum-phase transitions. Studying these emergent phenomena necessitates the preparation of large and high-quality single crystals. We report on the optimization of the single crystal growth for two Yb-based quantum critical materials, $YbRh_2Si_2$ and $YbNi_4P_2$. The prototype heavy-fermion system $YbRh_2Si_2$ is situated extremely close to an unconventional antiferromagnetic (AF) quantum critical point (QCP). The AF ordering (T_N = 70 mK) can be further lowered by chemically induced negative pressure using Ir-substitution. The QCP is reached for an Ir-substitution of x ≈ 0.1 in $Yb(Rh_{1-x}Ir_x)_2Si_2$ [1]. Here, we report on the optimization of the crystal growth of the substitution series as well as of the unsubstituted compound. We also report on our attempts to determine the melting point of $YbRh_2Si_2$ and present a phase analysis of the molten compound. In the heavy fermion metal, $YbNi_4P_2$, a ferromagnetic (FM) transition

at $T_C = 0.17$ K was observed recently and a FM QCP is reached at $x \approx 0.1$ in $YbNi_4(P_{1-x}As_x)_2$. We report on the crystal growth of $YbNi_4P_2$ by Czochralski method out of a Ni-P flux from a levitated melt. The obtained crystals were characterized by Laue X-ray scattering, X-ray powder diffraction, EDX microprobe analysis and resistivity measurements.

[1] S. Friedemann *et al.*, Nature Phys. **5**, 465 (2009).

TT 71.20 Wed 15:00 Poster B

Magnetic resonance in transverse-field Ising magnet LiHoF4 through quantum and thermal phase transitions — •Ivan Kovacevic, Peter Babkevich, Mingee Chung, Giovanni Boero, and Henrik Ronnow — Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, Switzerland

Coplanar resonators and vector network analyzer (VNA) were used to measure the susceptiblity in wide frequency range up to 6 GHz. The investigated temperatures from 0.2 K to 4.2 K and field range from 0 to 9 T cover the thermal transition into a ferromagnetically ordered phase below 1.53 K in zero-field as well as the quantum phase transition into a quantum-disordered paramagnetic phase above critical field 4.95 T at zero temperature. Entangled electro-nuclear states in LiHoF4 were probed by excitation field matching the hyperfine transitions at resonant frequencies. Absorption line was obtained by sweeping the transverse field at different frequencies. The model calculations within the mean-field approximation enable to track the evolution of the hyperfine levels as a function of field and temperature through quantum and thermal transitions, and show indeed excellent agreement with the experimental results. The presented methodology may find immediate applications to other important rare-earth containing materials such as spin ice, particularly close to the quantum phase transitions.

TT 71.21 Wed 15:00 Poster B

Thermodynamics of the Ising chain compound $CoNb_2O_6$ in transverse magnetic field — •Daniel Brüning[1], Simon Scharffe[1], Victoria Cho[1], Martin Valldor[1,2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

$CoNb_2O_6$ is a model system to investigate a quantum phase transition in magnetic fields. The structure consists of layers of CoO_6 octhahedrons separated by non-magnetic NbO_6 layers. The edge-sharing oxygen octahedrons link the Co^{2+}spins through Co-O-Co superexchange and form 1D ferromagnetic zigzag chains along the orthorhombic c axis. Crystal field effects lead to an easy-axis anisotropy of the Co^{2+} moments in the ac plane and to an effective spin-1/2 chain system described by the Ising model. A purely 1D Ising chain develops long-range order at zero temperature only and a transverse field induces a quantum phase transition into a quantum disordered state. Due to small inter-chain couplings $J_{||} \approx 0.01 \cdot J_{\perp}$, $CoNb_2O_6$ shows 3D long-range antiferromagnetic order below T_N=2.95 K. Because a magnetic field parallel to the b axis is normal to the easy-axis of the spin chain it is possible to study the complex interplay of 3D ordering and 1D quantum phase transitions. We present specific heat and magnetization measurements from about 0.3 to 10 K and discuss the phase diagram. The theoretical model of the Ising chain in transverse magnetic field is completely solvable and we compare our measurements to the corresponding calculations.

TT 71.22 Wed 15:00 Poster B

Ferromagnetic quantum critical point in $CeTi_{1-x}V_xGe_3$ — •Wolfram Kittler[1], Christian Taubenheim[1], Veronika Fritsch[1,2], Paul C. Canfield[3], and Hilbert v. Löhneysen[1] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, Germany — [2]Universität Augsburg, Institut für Physik, Experimentalphysik VI, Germany — [3]Ames Laboratory, US DOE, and Dept. of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA

$CeTiGe_3$ is a moderate heavy-fermion system, crystallizing in a hexagonal perovskite structure. It orders ferromagnetically at $T_C = 14.3$ K. Experiments on polycrystals have shown that the substitution of Ti with V suppresses the magnetic order, suggesting the existence of a ferromagnetic quantum critical point [1]. We have successfully grown single crystals of $CeTi_{1-x}V_xGe_3$. The strong uniaxial anisotropy with the easy axis along the c-axis is reduced with increasing x and turns into an easy ab-plane anisotropy for $x = 1$. The magnetic ordering temperature is indeed shifted to $T_C \to 0$ at a V concentration $x_c \approx 0.4$. We present data of magnetization, electrical resistivity and specific heat down to $T = 100$ mK of $CeTi_{1-x}V_xGe_3$. These data support the existence of a ferromagnetic quantum critical point.

[1] W. Kittler *et al.*, Phys. Rev. B **88**, 165123 (2013).

TT 71.23 Wed 15:00 Poster B

High-pressure transport properties of CrB_2 — •Alexander Regnat[1], Julian Becker[1], Jan Spallek[1], Andreas Bauer[1], Alfonso Chacon[1], Robert Ritz[1], Christian Blum[2], Sabine Wurmehl[2], and Christian Pfleiderer[1] — [1]Physik-Department, Technische Universität München, D-85748 Garching, Germany — [2]Leibniz Institute for Solid State and Materials Research IFW, D-01171 Dresden, Germany

High quality single crystals of the itinerant antiferromagnet CrB_2, $T_N = 88$ K, were grown by means of optical float zoning. Bulk, transport and de Haas-van Alphen measurements were carried out [1,2]. Here, we present a comprehensive study of the high-pressure transport properties. Samples were investigated under hydrostatic, uniaxial and quasi-hydrostatic conditions. As a result we are able to attribute contradictory reports for the pressure dependence of T_N to uniaxial strain [3, 4]. Perhaps most interestingly, we find a pronounced low temperature resistivity anomaly around 3 GPa in the quasi-hydrostatic case.

[1] Bauer et al., PRB 90, 064414 (2014).
[2] Brasse et al., PRB 88, 155138 (2013).
[3] Boeuf, PhD thesis (2003).
[4] Grechnev et al., J. Low Temp. Phys. 35, 531 (2009).

TT 71.24 Wed 15:00 Poster B

Impact of Local Magnetic Moments on the Anderson Metal-Insulator Transition — •Daniel Jung[1], Keith Slevin[2], and Stefan Kettemann[1] — [1]School of Engineering and Science, Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany — [2]Department of Physics, Graduate School of Science, Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan

We study the effects of classical magnetic impurities on the Anderson metal-insulator transition numerically. In particular we find that while a finite concentration of Ising impurities lowers the critical value of the site-diagonal disorder amplitude W_c, in the presence of Heisenberg impurities, W_c is first enhanced with increasing exchange coupling strength J due to time-reversal symmetry breaking. The resulting scaling with J is analyzed and compared to analytical predictions by Wegner [1]. The results are obtained numerically, based on a finite-size scaling procedure for the typical density of states, which is the geometric average of the local density of states. The latter can efficiently be calculated using the kernel polynomial method (KPM). We extend previous approaches by combining the KPM with a finite-size scaling analysis. We also discuss the relevance of our findings for systems like phosphor-doped silicon, which are known to exhibit a quantum phase transition from metal to insulator driven by the interplay of both interaction and disorder, accompanied by the presence of a finite concentration of magnetic moments.

[1] F. Wegner, Nucl. Phys. B 280, 210 (1987).

TT 71.25 Wed 15:00 Poster B

Suppression of critical fluctuations of electronic Ising-nematicity by coupling to the crystal lattice — •Christopher Max[1], Achim Rosch[1], Indranil Paul[2], and Markus Garst[1] — [1]Institute for theoretical Physics, Universitiy of Cologne, Zülpicher Str. 77, 50937 Cologne, Germany — [2]Laboratoire Matériaux et Phénomènes Quantiques, Université Paris Diderot-Paris 7 & CNRS, UMR 7162, 75205 Paris, France

Nematic instabilities of the electronic Fermi surface are relevant for various strongly-correlated systems like the ruthenates or the Fe-based superconductors. At the same time, they serve as a theoretical paradigm for quantum phase transitions in metals whose properties at lowest temperature still remain unclear and are the topic of current research. In the present work, we point out that the Ising-nematic order parameter strongly hybridizes with the strain field of the crystal, and, as a consequence, the nematic transition is naturally accompanied with a tetragonal-orthorhombic distortion. Due to the long-range shear forces of the crystal, the quantum critical properties will be eventually governed by quantum critical elasticity [1]. Upon approaching the quantum critical point, a crossover occurs from critical non-Fermi liquid behavior to conventional metallicity while the phonon sectors becomes soft resulting in an anomalous phonon specific heat $C_{ph} \sim T^{2.5}$ at lowest temperature. We discuss the various crossovers for thermodynamics as well as for the electronic spectral function.

[1] M. Zacharias, I. Paul and M. Garst, arXiv:1411.6925

TT 71.26 Wed 15:00 Poster B

Magnetic field and impurity studies in Kitaev and Kitaev Heisenberg models — •Sitikantha Das[1], Zhu Zengwei[2], Ross McDonald[2], Suchitra Sebastian[1], and Vikram Tripathi[3] — [1]Cavendish Labs, Cambridge — [2]National High Magnetic Field Laboratory, Los Alamos — [3]Tata Institute of Fundamental Research, Mumbai

In an effort to find an experimental realisation of Kitaev physics in solid state systems, the layered alkali iridates A_2IrO_3 (A = Li, Na), seem to be promising material candidates. Although the spin-1/2 Kitaev model has a quantum spin-liquid ground state with short ranged spin correlations and low-energy emergent excitations that are dispersing Majorana fermions, it has now been established that Na_2IrO_3 orders into a zig-zag state below 15 K. We have performed pulsed magnetic field torque experiments on Na_2IrO_3 at various field orientations and we observe strong angular dependence. Using negative Kitaev-Heisenberg as a model, we attempt to study the magnetisation and torque using exact diagonalization with a view to understand the experimental data.

We also study the effect of coupling an external magnetic impurity to a Kitaev model numerically. Antiferromagnetic coupling of the impurity spin results in the creation of finite flux excitations, which is now known from analytical calculations. This is verified numerically and we also study the effect of tuning the coupling strength from antiferromagnetic to ferromagnetic interaction.

TT 71.27 Wed 15:00 Poster B

The phase diagram of the XXZ model on the anisotropic triangular lattice — •Shijie Hu[1], Jize Zhao[2,3], Xuefeng Zhang[1], and Sebastian Eggert[1] — [1]Department of Physics and Research Center OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institute of Applied Physics and Computational Mathematics, Beijing 100088, China — [3]Beijing Computational Science Research Center, Beijing 100084, China

We use the density-matrix renormalization group (DMRG) in two dimensions to systematically study the full phase diagram of a general antiferromagnetic XXZ model on the anisotropic triangular lattice (called J_z-J_x-J'_z-J'_x model). In the strong-coupling limit of large J_z/J_x, we find a broad incommensurate supersolid phase in between the 1/2 filled Néel phase and 1D-decoupled-chain phase as a function of anisotropy. The incommensurate vector of this coplanar phase is related to the quantized density of domain walls along the vertical axis. In the other limit of large J_x/J_z, we find an incommensurate superfluid phase (cone phase). The transition region from supersolid phase to superfluid phase for intermediate coupling strength J_z/J_x, shows a rich physical behavior and provides a hint about the existence of a gapped 'spin-liquid' phase proposed by P. W. Anderson several decades ago.

TT 71.28 Wed 15:00 Poster B

Quantum Monte Carlo calculations for frustrated spin systems — Andreas Honecker[2], •Rene John Kerkdyk[1], Thomas Pruschke[1], and Stefan Wessel[3] — [1]Georg-August-Univesität Göttingen — [2]Université de Cergy-Pontoise, Laboratoire de Physique Théorique et Modélisation — [3]RWTH Aachen

Using Quantum Monte Carlo methods to examine the behavior of frustrated spin systems at low temperatures is usually problematic due to the sign problem. Our research focuses on a cluster approach to a model-specific elimination or reduction of the sign problem. We have implemented this approach in a worm algorithm for a one-dimensional spin-1/2 Heisenberg ladder and show that it permits access to the thermodynamic behaviour over the entire temperature range.

TT 71.29 Wed 15:00 Poster B

Optical absorption of the spin-1/2 Heisenberg antiferromagnet on a triangular lattice — •Boris Celan and Wolfram Brenig — Institute for Theoretical Physics, Technische Universität Braunschweig

We investigate the optical absorption of the spin-1/2 antiferromagnetic Heisenberg model on the two-dimensional anisotropic triangular lattice.

Vertex functions for the absorption of light are derived within a model of phonon-assisted multimagnon excitations and their momentum dependence is analyzed. For the magnetic excitations we use linear spin-wave theory. For the optical conductivity we derive a Bethe-Salpeter equation including quasi-particle renormalization and irreducible vertex functions to order 1/S. Numerical solutions of this integral equation are discussed on finite lattices up to 33x33 sites with and without final-state interactions.

We find the optical absorption to be qualitatively insensitive to the inclusion of final-state interactions. Results will also be presented for optical vs acoustic phonons. For low frequencies we derive asymptotic analytic expressions for the absorption which will be compared to our numerical results.

TT 71.30 Wed 15:00 Poster B

Insight in orbital resolution of lattice susceptibilities of strongly correlated electron systems — •Lewin Boehnke[1], Alexander Lichtenstein[2], Mikhail Katsnelson[3], and Frank Lechermann[2] — [1]University of Fribourg, Switzerland — [2]University of Hamburg, Germany — [3]University Nijmegen, The Netherlands

Recent advances in the numerical ascertainment of lattice susceptibilities of strongly correlated electron systems [1] in a rigorous manner on a similar footing as the dynamical mean field theory (DMFT) allow to step out of the comfort zone of a single orbital approximation to realistic materials.

Outside this zone, new challenges and opportunities lie in the physical interpretation of these versatile quantities.

We show the wave-vector dependent variation of orbital resolution of the magnetic susceptibility of Sr_2RuO_4, culminating in unexpected lack thereof at its incommensurate peak as well as the intrinsically non-local order parameter of the hidden-order phase in $LiVS_2$[2].

[1] Boehnke, Hafermann, Ferrero, Lechermann, Parcollet, PRB **84** (2011)

[2] Boehnke, Lichtenstein, Katsnelson, Lechermann, arXiv: 1407.4795 (2014)

TT 71.31 Wed 15:00 Poster B

High-temperature heat transport in spin-1/2 quantum magnets — •Christian Hess[1,2], Oleg Mityashkin[1], Ashwin Mohan[1], Chinnathambi Sekar[1], Gernot Krabbes[1], Sabine Wurmehl[1], Bernd Büchner[1,2], Romuald Saint-Martin[3], and Alexandre Revcolevschi[3] — [1]Institute for Solid State Research, IFW Dresden, 01069 Dresden, Germany — [2]Center for Transport and Devices, Technische Universität Dresden, 01069 Dresden, Germany — [3]Laboratoire de Physico-Chimie de L'Etat Solide, Université Paris-Sud, 91405 Orsay, France

Some years ago, a new, magnetic mode of heat transport has been discovered in low-dimensional spin-1/2 quantum magnets, i.e. spin planes, spin-ladders, and chains as realized in cuprate materials with large magnetic exchange $J/k_B \sim 2000$ K, and is intensely studied since then. The magnetic heat conductivity of such quantum magnet materials can be exceptionally large (even at room temperature), dwarfs the phonon heat conduction and thereby leads to an overall magnitude of the heat conductivity which can be comparable to that of metals. Here we present recent results which extend the accessible temperature range towards high temperature, approaching, for the first time, $k_BT \approx J/2$. The data provide fresh experimental input that allows to rationalize the high-temperature scattering processes for elementary excitations of the quantum magnets.

TT 71.32 Wed 15:00 Poster B

Crystal growth of frustrated materials with kagome-lattices — •Christian Klein, Pascal Puphal, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität, Frankfurt, Germany

Kagome-lattices are promising materials to investigate frustrated quantum spin systems with a possible quantum spin liquid (QSL) ground state [1]. High-quality single crystals are essential to distinguish between disordered magnetic ground-states and a true QSL.

We report on synthesis and characterization of the materials Herbertsmithite ($Cu_3Zn(OH)_6Cl_2$) and Barlowite($Cu_4(OH)_6BrF$), which represent model systems for two-dimensional Kagome-layered structures [2]. The kagome-layers are build up by copper ions and separated from each other through a transition-metal cation, so that a quasi-two-dimensional system is created [3]. Single crystals were grown under hydrothermal conditions.

We present the details of the crystal growth and preliminary substitution experiments to study their influence on the magnetic properties.

[1] P. A. Lee, Science 321, 1306 (2008).
[2] M. Shores et al., J. Am. Chem. Soc. 127, 13462 (2005).

[3] S. Chu et al., Appl. Phys. Lett. 98, 092508 (2011).

TT 71.33 Wed 15:00 Poster B

Spin dynamics in the kagome compound $YBaCo_3AlO_7$ — •M. Iakovleva[1,2], E. Vavilova[1,2], H.-J. Grafe[1], M. Valldor[3], V. Kataev[1], and B. Büchner[1] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Zavoisky Physical-Technical Institute, 420029 Kazan, Russia — [3]MPI CPfS, 01069 Dresden, Germany

$YBaCo_3AlO_7$ is a transition metal oxide compound with a magnetic kagome substructure where unconventional ground states such as a spin liquid can be expected. We have investigated the ground state and low energy spin dynamics of this material by ^{27}Al nuclear magnetic resonance spectroscopy.

The characteristic features of the spectral shape and of the relaxation rate temperature dependences show that short-range quasi static correlations occur in the system but not a long-range antiferromagnetic order. We compare our NMR results with AC and DC susceptibility measurements and discuss a possible realization of a spin glass state due to intrinsic structural disorder in this material.

TT 71.34 Wed 15:00 Poster B

NMR of the Shastry-Sutherland lattice $SrCu_2(BO_3)_2$ in pulsed magnetic fields — R. Stern[1], J. Kohlrautz[2], J. Haase[2], •H. Kuehne[3], E.L. Green[3], and J. Wosnitza[3] — [1]National Institute of Chemical Physics and Biophysics, 12618 Tallinn, Estonia — [2]Universität Leipzig, Faculty of Physics and Earth Sciences, 04103 Leipzig, Germany — [3]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

$SrCu_2(BO_3)_2$ is a quasi-two-dimensional spin system consisting of Cu^{2+} ions which form orthogonal spin-singlet dimers, also known as the Shastry-Sutherland lattice. This system has been studied extensively using a variety of techniques to probe the spin-triplet excitations, including recent magnetization measurements over 100 T. Spectroscopic techniques, such as nuclear magnetic resonance (NMR), can provide further insight into the spin-coupling mechanisms and excitations. We present ^{11}B NMR spectra measured in pulsed magnetic fields up to 54 T, and compare those with prior results obtained in static magnetic fields at 41 T. Herewith, we prove the feasibility and efficacy of this technique, yielding the capability for extended studies at highest magnetic fields up to the 100 T regime that determine the spin structure in the 1/3 magnetization plateau and beyond.

TT 71.35 Wed 15:00 Poster B

Scaling of the magnetic response in $YbCo_2Si_2$ — •A. Hannaske[1], K. Schmalzl[2], N. Mufti[1], C. Geibel[1], and O. Stockert[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]JCNS at ILL, Grenoble, France

$YbCo_2Si_2$ is a moderate heavy-fermion compound and orders antiferromagnetically below $T_N = 1.7$ K. In zero magnetic field two ordered phases occur. The low-temperature commensurate magnetic structure with an ordering wave vector $k = (0.25\ 0.25\ 1)$ can be continuously suppressed in a magnetic field $B||[1\bar{1}0]$ exhibiting a critical field $B_c(T_N = 0) = 2$ T where the transition to the paramagnetic phase takes place. Extensive inelastic neutron scattering experiments have been performed on singe-crystalline $YbCo_2Si_2$ at B_c as a function of temperature. The magnetic response of the ordering wave vector shows a critical slowing down when lowering the temperature down to zero indicating the proximity to quantum criticality. Furthermore, the response has been analyzed with respect to possible scaling behavior. Assuming a spin-density-wave scenario with three-dimensional quantum-critical spin fluctuations leads to a better collapse of all measured data points than a scenario with local critical fluctuations. This finding is in line with results of the specific heat, which doesn't show any sign of divergence at lowest T at the critical field B_c.

TT 71.36 Wed 15:00 Poster B

Pressure induced magnetic ordering in $SrCo_2P_2$ — •Helge Rosner, Sarah Ackerbauer, Christoph Bergmann, Moritz Besser, Michael Nicklas, and Christoph Geibel — MPI CPfS, Dresden, Germany

Since the discovery of superconductivity in doped iron pniktides, in particular the AFe_2As_2 systems of the $ThCr_2Si_2$ structure type, the intricate interplay of crystal structure, magnetism and superconductivity in these compounds has attracted broad attention. It is widely believed that the superconductivity of this compound family is closely related tho spin fluctuations. $SrCo_2P_2$ is a structural homologue of the AFe_2As_2 compound series, exhibiting a paramagnetic ground state, but in close vicinity to a quantum critical point. In our joined experimental and theoretical study we demonstrate that under hydrostatic pressure the system undergoes an isostructural transition to the so-called tetragonal collapsed state with a strongly reduced c/a ratio by about 15%. Surprisingly, this transition is accompanied by magnetic ordering, indicated by a magnetic-field-dependent kink in the resistivity. Our results are supported by density functional electronic structure calculations.

TT 71.37 Wed 15:00 Poster B

Tuning of the magnetic interactions in the frustrated spin chain compound linarite via hydrostatic pressure — •Jonathan Noky[1], Wolf Schottenhamel[1], Stefan-Ludwig Drechsler[1], Stefan Süllow[2], Anja U. B. Wolter[1], and Bernd Büchner[1] — [1]IFW Dresden, Dresden, Germany — [2]IPKM, TU Braunschweig, Braunschweig, Germany

Linarite ($PbCuSO_4(OH)_2$) is an anisotropic, quasi-one-dimensional frustrated spin-chain compound with competing ferromagnetic nearest-neighbor and antiferromagnetic next-nearest neighbor exchange interactions. Due to small but non-negligible interchain interactions linarite shows magnetic long-range order below T = 2.8K, where a helical ground state and a rich magnetic phase diagram have been observed for magnetic fields H parallel to the chain direction [1]. The magnetic interactions and thereby the frustration ratio strongly depends on the bond angles and bond lengths between involved copper and oxygen atoms. In order to systematically change them, the application of chemical or hydrostatic pressure is a powerful tool. We present a magnetization study of linarite under high hydrostatic pressures for different magnetic fields both perpendicular and parallel to the chain direction.

[1] B. Willenberg et al., Phys. Rev. Lett. 108, 117202 (2012).

TT 71.38 Wed 15:00 Poster B

Amorphous ferromagnetism and re-entrant magnetic glassiness in $Sm_2Mo_2O_7$ — •Giacomo Prando[1], Pietro Carretta[2], Anja Wolter-Giraud[1], Romuald Saint-Martin[3], Alexandre Revcolevschi[3], and Bernd Büchner[1,4] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany — [2]Dipartimento di Fisica e Unitá CNISM di Pavia, Universitá di Pavia, I-27100 Pavia, Italia — [3]Laboratoire de Physico-Chimie de l'Etat Solide, ICMMO, UMR8182, Université Paris-Sud, F-91405 Orsay, France — [4]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany

We report on the investigation of a high-quality single crystal of $Sm_2Mo_2O_7$ by means of dc magnetometry, muon spin spectroscopy and high-harmonics ac susceptibility [1]. The magnetic phase of the Mo^{4+} sublattice develops below $T_C = 78$ K and is typically discussed in the literature as a conventional itinerant ferromagnetic state. However, our results clearly detect a complicated superposition of conventional and highly disordered magnetic behaviors below 78 K sharing several common features with amorphous ferromagnetic alloys and with other insulating spin-glass pyrochlore molybdates. As typical for amorphous ferromagnets, a freezing of the transverse XY spin components of Mo^{4+} below $T \sim 25$ K is evidenced, an effect otherwise known as re-entrant spin-glass phase. Our results shed new light on the magnetic properties of $Sm_2Mo_2O_7$ and on the overall electronic phase diagram commonly accepted for pyrochlore molybdates.

[1] G. Prando et al., *Phys. Rev. B* **90**, 085111 (2014)

TT 71.39 Wed 15:00 Poster B

Local magnetic properties of diluted honeycomb iridates $Na_{3-\delta}M\mathbf{Ir_2O_6}$ (M = Zn, Cu, Ni) probed by ^{23}Na-NMR and μ^+SR — •Giacomo Prando[1], Evgeniya Vavilova[1,2], Alexey Alfonsov[1], Hans-Joachim Grafe[1], Vladislav Kataev[1], Bernd Büchner[1,3], Kristen Baroudi[4], Cindi Yim[4], John Roudebush[4], Huiwen Ji[4], and Robert Cava[4] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany — [2]Zavoisky Physical Technical Institute of RAS, Kazan, Russia — [3]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [4]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA

We present an experimental investigation of the magnetic properties of a series of sodium ternary iridates $Na_{3-\delta}MIr_2O_6$ (M = Zn, Cu, Ni) by means of local spin-probe techniques. In these materials, Ir ions are arranged in hexagonal honeycomb layers while the transition metal ions M substitute the Na ions in the hexagons center, with some detected

degree of M/Ir site mixing [1]. Together with our earlier magnetization measurements [1], our results give evidence that the doping of the Ir honeycomb lattice has a remarkable impact on the overall magnetic properties. In contrast to a well-defined long-range antiferromagnetic (AF) order in Na_2IrO_3, our data clearly reveal two different regimes at low temperatures, namely a static AF ordering and a spin glass behavior with short range spin correlations. The interplay and coexistence of these regimes depends on the specific element M.

[1] K. Baroudi et al., *Journ. Sol. State Chem.* **210**, 195 (2014)

TT 71.40 Wed 15:00 Poster B

Accessing the magnetic properties of iridium oxides by means of electron spin resonance — •Stephan Fuchs[1], Giacomo Prando[1], Alexey Alfonsov[1], Vladislav Kataev[1], Bernd Büchner[1,2], Brendan Phelan[3], and Robert Cava[3] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany — [2]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [3]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA

We report on our first results of electron spin resonance (ESR) measurements performed on exemplary iridium-based oxides. These are aimed at understanding the microscopic magnetic properties of these materials which are ultimately arising from a complex interplay of spin-orbital interactions and strong electronic correlations. $La_{11-x}Sr_xIr_4O_{24}$ allows us to detect single-iridium ion spectroscopic features thanks to the large distance among iridium-oxygen cages. At the same time, the increased inter-ions interactions in Na_2IrO_3 lead to a clear broadening of the ESR signal. We discuss our preliminary results in a wide range of temperatures and magnetic fields (up to 16 T).

TT 71.41 Wed 15:00 Poster B

Hydrostatic pressure experiments on frustrated hexagonal Iridates — •Rudra Sekhar Manna, Friedrich Freund, and Philipp Gegenwart — EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany

Hexagonal iridates A_2IrO_3 (A = Na, Li) have novel electronic and magnetic properties due to the strong spin-orbit coupling and electronic correlations. They are proposed candidate materials for the realization of the frustrated bonding-dependent anisotropic Kitaev interaction [1, 2]. While the structure of Na_2IrO_3 and α-Li_2IrO_3 consists of a two-dimensional (2D) honeycomb lattice, a 3D, so-called hyper-honeycomb structure is realized in β-Li_2IrO_3 [3, 4]. All different materials display long-range magnetic order, in contrast to a Kitaev quantum spin-liquid, although the analysis of the magnetic properties indicates dominating Kitaev exchange interactions [3]. The Kitaev interaction sensitively depends on the Ir-O-Ir bonding angle which may be varied by external pressure. This motivates a detailed study of the hydrostatic pressure dependence of the magnetic properties of hexagonal iridates. In particular we investigate the bulk magnetization in a commercial SQUID magnetometer up to 2 GPa using Daphne oil as pressure medium and a small piece of lead as pressure sensor.

[1] Y. Singh *et al.*, PRL **108**, 127203 (2012).
[2] S. Manni *et al.*, PRB **89**, 245113 (2014).
[3] A. Biffin *et al.*, PRB **90**, 205116 (2014).
[4] T. Takayama *et al.*, arXiv:1403.3296 (2014).

TT 71.42 Wed 15:00 Poster B

Possibility of a two-dimensional spin liquid in CePdAl induced by partial geometric frustration? — •V. Fritsch[1,2], K. Grube[2], W. Kittler[2], C. Taubenheim[2], Z. Huesges[3], S. Lucas[3], E. Green[4], O. Stockert[3], and H. v. Löhneysen[2] — [1]Universität Augsburg, Institut für Physik, Experimentalphysik VI, Germany — [2]Karlsruher Institut für Technologie, Germany — [3]Max-Planck-Institut für chemische Physik fester Stoffe, Dresden, Germany — [4]Hochfeldzentrum Dresden-Rossendorf, Germany

CePdAl crystallizes in the hexagonal ZrNiAl structure, where the magnetic ions form a distorted kagomé lattice. At $T_N = 2.7$ K the onset of antiferromagnetic (AF) order is observed. Neutron scattering experiments [1] revealed a partial frustration in the distorted kagomé planes of this structure: two-thirds of the Ce moments form ferromagnetic chains, which are antiferromagnetically coupled, the remaining third do not participate in any long-range order. Along the c-axis the magnetic moments exhibit an amplitude modulation. Accordingly, the kagomé planes are stacked on top of each other, resulting in corrugated AF planes parallel to the c-axis formed by the ordered magnetic moments, which are separated by the frustrated moments [2]. It is an intriguing and yet unresolved question if this third of frustrated moments forms a spin liquid state in CePdAl. Based on measurements of specific heat, thermal expansion, magnetization and electrical resistivity we want to discuss this possibility.

[1] A. Dönni *et al.*, J. Phys.: Condens. Matter **8**, 11213 (1996).
[2] V. Fritsch *et al.*, Phys. Rev. B **89**, 054416 (2014).

TT 71.43 Wed 15:00 Poster B

Dielectric measurements of magnetic monopoles on the spin-ice compounds $(Ho/Dy)_2Ti_2O_7$ — •Manuel Pietsch, Christoph P. Grams, Jean-Francois Welter, Victoria Cho, Thomas Lorenz, and Joachim Hemberger — II. Physikalisches Institut, Universität zu Köln, Cologne, Germany

In so-called spin-ice compounds a frustrated ground-state with finite zero-point entropy is stabilized via competing interactions and emergent magnetic monopoles excitations [1]. It was postulated that a magnetic monopole holds an electric dipole moment [2], which allows to investigate their dynamics via the dielectric function $\varepsilon(\nu)$.

In $Dy_2Ti_2O_7$ a critical speeding-up for frequencies up to 100 kHz was reported down to temperatures of 200 mK with a specific focus on the critical endpoint present for a [111] magnetic field [3]. In $Ho_2Ti_2O_7$ both faster relaxation dynamics compared to the sister-compound and an additional relaxation process are suspected [4].

Here we report on broadband dielectric spectroscopy measurements of $\varepsilon(\nu)$ in $Ho_2Ti_2O_7$.

Funded through the Institutional Strategy of the University of Cologne within the QM2 Excellence Initative and research grant HE-3219/2-1.

[1] C. Castelnovo et al., Nature 451 (2008) 42
[2] D. I. Khomskii, Nature Comm. 3 (2012) 1
[3] C.P. Grams et al., Nature Comm. 5 (2014) 4853
[4] G. Ehlers et al., J. Phys.: Cond. Mat. 16 (2004) S635

TT 71.44 Wed 15:00 Poster B

Heat Transport in dilute Spin-Ice Materials $(R_{1-x}Y_x)_2Ti_2O_7$ with R = Ho,Dy — •Jean-Francois Welter[1], Simon Scharffe[1], Gerhard Kolland[1], Martin Valldor[1,2], Victoria Cho[1], Peter Laschitzky[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Max-Planck Institut für Chemische Physik fester Stoffe, Dresden, Germany

In the spin-ice materials $R_2Ti_2O_7$ the magnetic R^{3+} ions form a network of corner-sharing tetrahedra. Recently, these materials attracted a lot of interest due to their groundstate degeneracy and the description of the low-energy excitations as magnetic monopoles[1]. In order to investigate the influence of the monpole propagation on the thermal conductivity κ, we dilute the spin-ice compounds with non-magnetic Yttrium. We synthesized single crystals of the series $(R_{1-x}Y_x)_2Ti_2O_7$ with $0 \leq x \leq 0.75$ using the floating-zone method. Comparing the thermal conductivity for different doping levels x, the total κ can be separated into a sum of phononic (κ_{ph}) and magnetic (κ_{mag}) contributions. In both $R_2Ti_2O_7$ compounds, κ_{mag} is sizable and can be attributed to magnetic monopole excitations[2]. We find that κ_{mag} is more pronounced in $Dy_2Ti_2O_7$ and that the field dependences of κ_{ph} are of opposite signs in the Dy- and Ho-based materials[3].

This work was supported by DFG via the project LO 818/2-1.

[1] Castelnovo *et al.*, Nature **451**, 42 (2008).
[2] Kolland *et al.*, Phys. Rev. B, **86**, 060402(R) (2012).
[3] Scharffe *et al.*, J. Magn. Magn. Mater. (in press, arXiv:1406.4037).

TT 71.45 Wed 15:00 Poster B

Influence of Ti deficiency on the magnetic properties in $Yb_2Ti_2O_7$ — •Marcel Naumann[1], Elizabeth L. Green[1], Sergei Zherlitsyn[1], Salim Erfanifam[1], Shadi Yasin[1], Joachim Wosnitza[1], Andrej Maljuk[2], Christian G. F. Blum[2], Rhea Kappenberger[2], Jan Trinckauf[2], Bernd Büchner[2], Sabine Wurmehl[2], Rajib Sarkar[3], Sirko Kamusella[3], Philipp Materne[3], Hans-Henning Klauss[3], Hubertus Luetkens[4], and Chris Baines[4] — [1]Hochfeld-Magnetlabor Dresden, HZDR, 01328 Dresden, Germany — [2]IFW, 01171 Dresden, Germany — [3]TU Dresden, 01069 Dresden, Germany — [4]PSI, 5232 Villigen, Switzerland

Frustrated spin systems with pyrochlore lattice exhibit a wide range of physical phenomena such as magnetic monopoles and residual entropies. In particular, $Yb_2Ti_2O_7$ has attracted attention in recent years, also due to the sample dependence of its ground state. While some works suggest a ferromagnetic ground state others see no long-

range magnetic ordering or spin freezing whatsoever.

We investigated two different samples grown under similar growth conditions using heat-capacity, ultra-sound, and μSR measurements. While one sample showed a crossover around 240 mK,the other exhibited no evidence of long-range magnetic order down to 15 mK. The results of subsequent x-ray and EDX measurements indicate a strong influence of Ti deficiency on the low-temperature magnetic properties. This offers a new tuning parameter for the ongoing search for a quantum spin liquid.

TT 71.46 Wed 15:00 Poster B

Phase separation in $Y_{0.63}Ca_{0.37}TiO_3$ — •Bernhard Zimmer[1], Raphael German[1], Thomas Koethe[1], Alexander Komarek[1,2], Markus Braden[1], and Paul van Loosdrecht[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

We have investigated the domain structure and Raman response of $Y_{0.63}Ca_{0.37}TiO_3$ single crystals which show a clear metal-to-insulator transition at ca. 170 K, with a wide hysteresis in the resistivity ranging down to ca. 50 K. We observe by use of a conventional optical microscope the appearance of two distinct regions at temperatures below ca. 200 K, with a characteristic length scale of order of 10 μm. By means of Raman spectroscopy we can identify the regions to correspond to the metallic and insulating domains, and follow the evolution of the domains as function of temperature down to 5 K.

TT 71.47 Wed 15:00 Poster B

Ultrasonic investigation of GaV_4S_8 — •P. T. Cong[1], S. Mombetsu[1,2], V. Tsurkan[3], A. Loidl[3], S. Zherlitsyn[1], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Department of Physics, Hokkaido University, Japan — [3]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

In recent years, transition metal-chalcogenides with the cubic $GaMo_4S_8$-type structure have attracted much interest because of their fascinating properties such as superconductivity under pressure, metal-insulator transition, 4*d* ferromagnetism and various structural and magnetic instabilities at low temperatures. These phenomena reflect the strong coupling of structural, electronic and magnetic degrees of freedom in this system. Here, we present results of ultrasound investigations performed on a high-quality single crystal of the tetrahedral magnetic-cluster material GaV_4S_8. The temperature dependence of the sound velocity and attenuation shows a huge anomaly at $T_s = 44$ K followed by a pronounce feature at $T_c = 12.5$ K related to a structural transition and ferromagnetic ordering, respectively, as known from previous magnetic-susceptibility and specific-heat results [1]. A field-induced transition at temperatures below T_c reveals a complex magnetic structure of GaV_4S_8, suggesting a competition of several interactions. Based on these measurements, we mapped out the $B-T$ phase diagram of GaV_4S_8 and discuss the role of the lattice degrees of freedom in this material.

[1] H. Nakamura et al., J. Phys.: Condens. Matter 17, 6015 (2005)

TT 71.48 Wed 15:00 Poster B

Skyrmion density correlations in critical chiral paramagnets — •Laura Köhler, Achim Rosch, and Markus Garst — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

The interactions between critical paramagnons in chiral magnets like MnSi or Cu_3OSeO_3 suppress the critical temperature and, in addition, drive the transition weakly first-order. Within the resulting fluctuation-disordered regime strong correlations prevail that substantially renormalize the correlation length in quantitative agreement with Brazovski theory [1,2,3]. Within this regime, we theoretically address the correlations of the skyrmion density that can be identified with the local vector chirality of the magnetization. These correlations are expected to be particularly pronounced for finite magnetic fields close to the skyrmion crystal phase. We compute the corresponding correlation function within the Brazovski approximation with the aim to identify additional microwave resonances.

[1] M. Janoschek *et al.* Phys. Rev. B **87**, 134407 (2013).
[2] A. Bauer *et al.*, Phys. Rev. Lett. **110**, 177207 (2013).
[3] J. Kindervater *et al.* Phys. Rev. B **89**, 180408(R) (2014).

TT 71.49 Wed 15:00 Poster B

Scattering of high-energy magnons from a magnetic skyrmion — •Sarah Schroeter and Markus Garst — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

The skyrmion is a topologically stable soliton solution in chiral magnets and corresponds to a large-amplitude excitation of the field-polarized ground state. We consider the fluctuation spectrum around such a soliton with particular focus on the scattering of high-energy magnons. The topological winding number of the skyrmion results in a finite Aharanov-Bohm flux density in the scattering potential that leads to skew and rainbow scattering of magnons [1]. We consider the differential cross section and the magnon pressure on the skyrmion within a semiclassical approximation and derive their high-energy asymptotics.

[1] C. Schütte and M. Garst, Phys. Rev. B 90, 094423 (2014).

TT 71.50 Wed 15:00 Poster B

Magnon excitations of magnetic helices and skyrmion crystals — •Johannes Waizner and Markus Garst — Institute for Theoretical Physics, Universität zu Köln, Köln, Germany

In chiral magnets long-range ordered magnetic crystals form with a lattice spacing proportional to the inverse of spin-orbit coupling. The magnetic helix corresponds to a one-dimensional crystal while the skyrmion lattice effectively realizes a two-dimensional magnetic crystal. We study the magnon excitations of these crystals that experience a characteristic Bragg scattering off their periodicity resulting in magnon band structure. For the helix, in particular, this leads to gaps in the spectrum that prohibit magnon propagation along the pitch direction. We also compare with recent results of inelastic neutron scattering [1].

[1] M. Kugler, G. Brandl, R. Georgii, K. Seemann, M. Janoschek, J. Waizner, M. Garst, A. Rosch, C. Pfleiderer, and P. Böni (unpublished)

TT 71.51 Wed 15:00 Poster B

Critical behavior of collective GHz excitations of Skyrmions and spin helices — •Ioannis Stasinopoulos[1], Stefan Weichselbaumer[1], Thomas Schwarze[1], Andreas Bauer[2], Helmuth Berger[3], Johannes Waizner[4], Markus Garst[4], Christian Pfleiderer[2], and Dirk Grundler[1,5] — [1]Physik-Department E10, TU München, Garching, Germany — [2]Physik-Department, FG Magnetische Materialien, TU München, Garching, Germany — [3]EPFL, Institut de physique de la matiere complexe, Lausanne, Switzerland — [4]Institute for Theoretical Physics, Univ. Köln, Köln, Germany — [5]IMX, EPFL, Lausanne, Switzerland

Skyrmions are topologically stable spin textures with the spins pointing in all directions wrapping up a sphere. They emerge in chiral-magnets, e.g. MnSi, and arrange in a hexagonal lattice with typical lattice constants of several tens of nm. Our group uses an all-electrical microwave spectroscopy setup based on a vector analyzer and lithographically fabricated coplanar waveguides to excite and simultaneously probe the spin states. We study and compare the temperature dependence of the dynamics both in the ordered magnetic phases and the regime just above T_c. This study addresses the dynamics of a suspected "Skyrmion liquid" above T_c and aims ultimately at deepening the microscopic understanding of crystallization processes in magnetism. Financial support by the DFG via TRR80 and NIM is acknowledged.

TT 71.52 Wed 15:00 Poster B

Collective GHz excitations of Skyrmions and spin helices in Cu_2OSeO_3 — •Stefan Weichselbaumer[1], Ioannis Stasinopoulos[1], Andreas Bauer[2], Helmuth Berger[3], Johannes Waizner[4], Markus Garst[4], Christian Pfleiderer[2], and Dirk Grundler[1,5] — [1]Physik-Department E10, TU München, Garching, Germany — [2]Physik-Department, FG Magnetische Materialien, TU München, Garching, Germany — [3]EPFL, Institut de physique de la matiere complexe, Lausanne, Switzerland — [4]Institute for Theoretical Physics, Univ. Köln, Köln, Germany — [5]IMX, EPFL, Lausanne, Switzerland

Skyrmions are topologically stable spin textures with the spins pointing in all directions wrapping up a sphere. We investigate collective excitations of Skyrmions and spin helices in the GHz-regime in the insulating multiferroic Cu_2OSeO_3. Using an all-electrical microwave spectroscopy setup based on a vector analyzer and lithographically fabricated coplanar waveguides (CPW) we excite and simultaneously probe the dynamics. By modifying the sample shape, CPW design, and excitation configuration, we address the dynamic modes differently. We compare our results with a mean-field theory taking into account dipolar interaction between the spins. The control over the dynamics opens the way towards helimagnet-based high-frequency de-

vices. Financial support by the DFG via TRR80 is acknowledged.

TT 71.53 Wed 15:00 Poster B

Corbino resistance measurements of the cubic helimagnet MnSi — •Marco Halder, Christoph Schnarr, Andreas Bauer, and Christian Pfleiderer — Technische Universität München, Physik-Department E21, D-85748 Garching, Germany

In recent years the transport properties of the itinerant helimagnet MnSi were heavily investigated. In particular, the topological Hall contribution arising from a regular arrangement of spin whirls, the so-called Skyrmion lattice, attracted great scientific interest. In addition, it was shown that already ultra-low current densities are sufficient to move the magnetic texture leading to emergent electrodynamics. Here, we report measurements on a disk-shaped sample with a coaxial contact arrangement, i.e., in a Corbino geometry, addressing geometrical contributions to the magnetoresistance of MnSi. We report the Corbino resistance of high-quality single crystals of MnSi over a wide range of temperatures from 2 K to 300 K under magnetic fields up to 9 T.

TT 71.54 Wed 15:00 Poster B

Chiral fluctuations in Cu_2OSeO_3 and FeGe in their field modulated states: ^{63,65}Cu and ^{57}Fe NMR study — •Mayukh Majumder, Hiroshi Yasuoka, Panchanan Khuntia, Markus Schmidt, and Michael Baenitz — Max Plank Institute for Chemical Physics of Solids, Dresden, Germany

Insulating Cu_2OSeO_3 (ferrimagnetic transition temperature at 58 K) and metallic FeGe (ferromagnetic transition temperature at 280 K) show different field modulated states such as helical, conical along with topological Skyrmion phase [1,2,3]. We employed ^{63,65}Cu and ^{57}Fe NMR as a on site probe of field modulated states. The evolution of spectral shape from helical to conical to ferrimagnetic (for Cu_2OSeO_3) or ferromagnetic state (for FeGe) have been investigated. Further the spin-lattice relaxation rate ($1/T_1$) and spin-spin relaxation rate ($1/T_2$) provide the nature of chiral spin excitations across different field modulated phase boundaries.

[1] Science 336, 198(2012).
[2] Phys. Rev. Lett. 107, 127203(2011).
[3] Nature 8 153(2013).

TT 71.55 Wed 15:00 Poster B

Pressure induced insulator-to-metal transition in $FePS_3$ — •Matthew John Coak[1], Charles Robert Sebastian Haines[1,2], and Siddarth Shankar Saxena[1] — [1]Cavendish Laboratory, University of Cambridge — [2]CamCool Research Ltd UK

$FePS_3$ is structurally and magnetically two-dimensional, with a magnetic ground state in which spins are ordered as ferromagnetic chains coupled antiferromagnetically. At ambient pressure, it is an insulator with a direct gap of approximately 0.5 eV and a room temperature resistivity of approximately 104 Ωcm. We present the results of exploratory resistivity, magnetisation and dielectric measurements under pressure for this material. The insulating phase is suppressed at a pressure in the range 40-70 kbar giving way to a new metallic phase. As yet unexplained intermediate behaviour is seen at pressures around the transition. At high pressure, the resistivity develops linear temperature dependence similar to that observed in Cuprates. At lower temperature, there is an upturn in resistivity which may indicate a low temperature phase transition or impurity scattering.

TT 71.56 Wed 15:00 Poster B

Field-dependent de Haas-van Alphen frequencies in the non-centrosymmetric compound CrGe — •J. Klotz[1,2], K. Götze[1,2], J. Bruin[3], C. Geibel[4], H. Rosner[4], K. Weber[4], M. Schmidt[4], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]High Magnetic Field Laboratory, Radboud University, Netherlands — [4]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

CrGe is a transition-metal germanide with the B20 non-centrosymmetric cubic structure. It does not exhibit any magnetic order in fields up to 60 T but the temperature dependence of the susceptibility and resistivity indicate its proximity to ferromagnetism [1]. Since CrGe has no inversion symmetry, it was expected to exhibit anti-symmetric spin-orbit interaction with split dHvA frequencies which are field dependent [2]. We present dHvA-effect data that were obtained employing rotatable capacitive torque magnetometers in a 18 T/30 mK and a 33 T/340 mK system. We found a clear field dependence of the dHvA frequencies as well as enlarged effective masses as was expected from the enhanced Sommerfeld coefficient of $\gamma = 19$ mJ/mol K^2

[1] T. Sato and M. Sakata, J. Phys. Soc. Jpn. **52** (1983), 1807
[2] V. P. Mineev and K. V. Samokhin, Phys. Rev. B **72** (2005), 212504.

TT 71.57 Wed 15:00 Poster B

Resistivity of MnB_4 — •Nico Steinki[1], Dirk Schulze Grachtrup[1], Stefan Süllow[1], Arno Knappschneider[2], and Barbara Albert[2] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, TU Darmstadt, Germany

In an effort to develop super hard materials, MnB_4 was recently synthesized for the first time in single crystalline form, with micro scale crystals of about 200 μm length. Subsequently, the magnetic properties have been studied experimentally, and band structure calculations have been carried out [1,2]. Based on these calculations and preliminary resistivity measurements, it was argued that the material is semiconducting, although a definite conclusion could not be reached.

In order to determine whether MnB_4 is a semiconductor or a metal we have carried single crystal resistivity measurements at temperatures 2 to 300 K. For this purpose a setup for measuring micro-scale samples was developed and characterized. The setup is based on a modified two point configuration and the resistivity of MnB_4 was measured as function of temperature. With these measurements MnB_4 was identified to be a semiconductor.

[1] A. Knappschneider et al., Angew. Chem. **126** (2014) 1710
[2] H. Gou et al., Phys. Rev. B **89** (2014) 064108

TT 71.58 Wed 15:00 Poster B

Signatures of the magnetostructural phase transition in CrN probed by temperature-dependent infrared spectroscopy — •Jihaan Ebad-Allah[1,2], Benjamin Kugelmann[1], Francisco Rivadulla[3,4], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Department of Physics, University of Tanta, 31527 Tanta, Egypt — [3]Center for Research in Biological Chemistry and Molecular Materials, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain — [4]Department of Physical Chemistry, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain

During the last decades, CrN has attracted great interest due to its superior high-temperature oxidation resistance, hardness, wear and corrosion resistance, and good chemical and thermal stability. In addition, CrN has remarkable electronic, optical, and magnetic properties. At the Neel temperature (T_N= 273-286 K) CrN undergoes a paramagnetic to antiferromagnetic phase transition, concomitant with a structural distortion from cubic rock-salt to orthorhombic [1].

We carried out temperature-dependent absorption measurements on CrN powder in the frequency range 250-7500 cm^{-1}. At ambient conditions, the absorption spectrum shows a phonon mode in the far-infrared range, a strong absorption band at around 0.17 eV, and a charge gap at ≈ 0.7 eV [2]. Below T_N, the phonon mode splits and the absorption edge shows a slight blue shift.

[1] A. Filippetti et al., Phys. Rev. B **59**, 7043 (1999).
[2] D. Gall et al., J. Appl. Phys. **91**, 5882 (2002);
A. Herwadkar et al.,Phys. Rev. B **79**, 035125(2009).

TT 71.59 Wed 15:00 Poster B

Influence of doping and quasi-lowdimensionality on the thermoelectric properties of strongly correlated materials — •Raphael Richter[1], Lewin Boehnke[2], Daniel Grieger[3], and Frank Lechermann[1] — [1]1. Institut fur Theoretische Physik, Universität Hamburg, Germany — [2]Département de Physique, University of Fribourg, Switzerland — [3]International School for Advanced Studies (SISSA), Trieste, Italy

Strongly correlated materials are among the most interesting and complicated systems in condensed matter physics. Large Seebeck coefficients are found in some of these compounds, which highlight the possibility for thermoelectric applications.

In this work, we study the thermoelectric properties of such systems by means of the charge self-consistent density functional theory (DFT) plus dynamical mean-field theory (DMFT) scheme, build on a mixed basis pseudopotential framework combined with a continuous time quantum Monte-Carlo solver. By means of this methodology we consider doping effects by constructing pseudopotentials with frac-

tional nuclear charge or within a supercell approach. For the investigation of the thermoelectric response, the (anisotropic) Seebeck tensor is calculated within the Kubo formalism at different temperatures.

TT 71.60 Wed 15:00 Poster B

Matrix-product-state method with local basis optimization for bosonic systems out of equilibrium — •Christoph Brockt[1], Eric Jeckelmann[1], Florian Dorfner[2], Lev Vidmar[2], and Fabian Heidrich-Meisner[2] — [1]Leibniz Universität Hannover, Germany — [2]Ludwig-Maximilians-Universität München, Germany

We present a method for simulating the time evolution of quasi-one-dimensional correlated systems with bosonic degrees of freedom using matrix product states. Our goal is the accurate description of systems with large bosonic fluctuations for long periods of time. For this purpose we combine the time-evolving block decimation (TEBD) algorithm [1] with a local basis optimization approach which yields so-called optimal boson states [2]. We discuss the performance of this approach in comparison to TEBD with a bare boson basis, exact diagonalizations, and diagonalizations in a limited functional space. First, we test our method for the non-equilibrium dynamics of a Holstein polaron [3] and show that it allows us to study the regime of strong electron-phonon coupling. Second, the method is applied to the scattering and self-trapping of an electronic gaussian wave packet traveling through a quantum wire with electron-phonon coupling. Support from the DFG through the Research Unit FOR 1807 is gratefully acknowledged.

[1] G. Vidal, PRL **93**, 040502 (2004)
[2] C. Zhang, E. Jeckelmann, and S.R. White, PRL **80**, 2661 (1998)
[3] F. Dorfner et al., arXiv:1411.5074 (2014)

TT 71.61 Wed 15:00 Poster B

Nonlinear charge transport in interacting ring structures: transient and steady state dynamics — •Benedikt Schönauer and Peter Schmitteckert — Institut für Nanotechnologie, Karlsruher Institut für Technologie, Karlsruhe, Deutschland

We investigate the effect of density-density interactions in various ring structures coupled to non-interacting leads on the transient and the steady state currents. To this end we use a time dependent density matrix renormalization group method to calculate the time resolved current in response to a quench in the charge balance. Our results suggest that an asymmetry of the ring structures gives rise to interesting new features of the long time limit of the local current in the rings. In addition finite size effects seem to be significantly increased for these systems as compared to strictly one-dimensional structures.

TT 71.62 Wed 15:00 Poster B

Time-dependent Gutzwiller wave function for the finite-dimensional Hubbard model in nonequilibrium — •Marc Alexander and Marcus Kollar — Theoretische Physik III, Universitität Augsburg

We apply the time-dependent Gutzwiller wave function (GWF) to the fermionic Hubbard model in nonequilibrium in two and three dimensions. For this purpose we combine two variational formalisms for the GWF, one that starts from the limit of infinite dimensions [1] and one that applies in arbitrary dimensions [2]. Similar to the one- and infinite-dimensional case, the resulting equations of motion are conservative and yield oscillatory behavior for an interaction quench, which we compare with the prethermalization dynamics on short timescales.
[1] M. Schiró and M. Fabrizio, Phys. Rev. Lett. **105**, 076401 (2010).
[2] M. Kollar and C. Gramsch, see Talk in TT.

TT 71.63 Wed 15:00 Poster B

Bound state fragmentation of a spin line in 2 dimensions — •Jonathan Lux and Achim Rosch — Institute for theoretical Physics, Cologne

We investigate the dynamics of a line of down-spins embedded in the ferromagnetic spin-up ground state of a two-dimensional XXZ model close to the Ising limit. We treat the system as an open 1 dimensional system, and use a Schrieffer Wolff transformation in combination with a semiclassical approximation to tackle this quantum quench problem. During the time evolution, the line is fragmented into free and bound states of down-spins. We determine the statistics of the bound states, which, in principle, can be measured in cold atom systems using a quantum microscope.

TT 71.64 Wed 15:00 Poster B

Enforcing conservation laws in nonequilibrium cluster perturbation theory — •Christian Gramsch and Michael Potthoff — I. Institute for Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany

Recently it has been proposed to solve the nonequilibrium Dyson equation by numerically decomposing the self-energy into its Lehmann representation [1]. This allows to replace the interaction term in the Hamiltonian by noninteracting bath degrees of freedom. In our present work we analytically construct the Lehmann representation of the self-energy for arbitrary interacting systems. For any finite system, e.g. a cluster system, the number of resulting noninteracting bath sites is finite. While this can already be used to solve nonequilibrium cluster perturbation theory (NE-CPT) [2] for arbitrary long times, we improve upon NE-CPT by enforcing local continuity equations for density and energy to be respected. Total energy and particle number are then conserved during the time evolution.

[1] K. Balzer and M. Eckstein, Phys. Rev. B 89, 035148 (2014)
[2] M. Balzer and M. Potthoff, Phys. Rev. B 83, 195132 (2011)

TT 71.65 Wed 15:00 Poster B

Quench dynamics studied by means of non-equilibrium self-energy-functional theory — •Felix Hofmann[1], Martin Eckstein[2], and Michael Potthoff[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, Universität Hamburg - CFEL

The non-equilibrium self-energy-functional theory (SFT) [1] provides a general framework for the systematic construction of non-perturbative approximations to study strongly correlated systems out of equilibrium. On the space of non-equilibrium self-energies, given on the Keldysh-Matsubara contour, the grand potential can be written as a functional which is stationary at the physical non-equilibrium self-energy. The corresponding variational principle is exploited by restricting the variations to variations of self-energies that are generated by an exactly solvable reference system.

Here we present first results obtained for Hubbard models where the real-time dynamics is induced by a quantum quench of the interaction parameter and using different reference systems. We discuss the details of the numerical implementation, present internal consistency checks, discuss the total energy conservation, and compare with literature data from the non-equilibrium dynamical mean-field theory.

[1] F. Hofmann, M. Eckstein, E. Arrigoni, and M. Potthoff, PRB 88, 165124 (2013)

TT 71.66 Wed 15:00 Poster B

Nonequilibrium Green functions approach to transport properties in strongly coupled finite quantum systems — •Niclas Schlünzen, Sebastian Hermanns, and Michael Bonitz — ITAP, Christian–Albrechts–Universität Kiel, Leibnizstr. 15, 24098 Kiel, Germany

Transport properties of strongly correlated quantum systems are of central interest in condensed matter, ultra-cold atoms and in dense plasmas[1]. There, the proper treatment of strong correlations is important. This can be achieved by using the nonequilibrium Green functions framework with a suitable chosen many-body approximation. In this contribution, we study transport properties of finite spatially inhomogeneous Hubbard systems with the T-matrix approximation[2]. The diffusion is analyzed for different spatial geometries in one to three dimensions as a function of the particle number and interaction strength.

[1] Balzer et al., Phys.Rev. B **79** 245306 (2009).
[2] Bonitz et al., Contrib.Plasma Phys. (2014), DOI: 10.1002/ctpp.201400065

TT 71.67 Wed 15:00 Poster B

Correlated lattice systems far from equilibrium—a nonequilibrium Green functions approach — •Sebastian Hermanns, Niclas Schlünzen, and Michael Bonitz — ITAP, Christian–Albrechts–Universität Kiel, Leibnizstr. 15, 24098 Kiel, Germany

The study of dynamical processes in lattice systems reveals a great variety of electronic phenomena which occur on an ultrafast time scale[1]. They include the build-up of inter-particle correlation as well as dynamically screening of the interaction. To describe these processes theoretically, the framework of non-equilibrium Green functions is very well suited. It provides a controlled way to generate various classes of many-body approximations focussed on different aspects of the experiment. In this contribution, we analyze the specific features covered

by the second order Born, GW and T-matrix approximation in combination with the Generalized Kadanoff-Baym ansatz [2] for Hubbard systems in arbitrary dimensions in nonequilibrium.

[1] Kajala et al., Phys.Rev.Lett. **106** 206401 (2011).
[2] Hermanns et al., Phys.Rev. B **90** 125111 (2014).

TT 71.68 Wed 15:00 Poster B

Nonlocal quantum kinetic theory — •Klaus Morawetz[1,2,3] and Pavel Lipavsky[4] — [1]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics (IIP), Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — [3]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [4]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

A quantum kinetic equation of nonlocal and non-instantaneous character is derived which unifies the achievements of the transport in dense quantum gases with the Landau theory of quasiclassical transport in dense Fermi systems. The numerical solution is not more expensive than solving the Boltzmann equation since large cancellations in the off-shell motion appear which are hidden usually in non-Markovian behaviors. The balance equations for the density, momentum and energy include quasiparticle contributions and the correlated two-particle contributions beyond the Landau theory. The medium effects on binary collisions are shown to mediate the latent heat, i.e., an energy conversion between correlation and thermal energy.

[1] V. Špička, P. Lipavský, K. Morawetz,
Phys. Rev. B. **55**, 5084 (1997); 5095 (1997)
[2] K. Morawetz, V. Spička, P. Lipavský, H.N. Kwong,
Phys. Rev. **C 59**,6 (1999) 3052-3059;
[3] P. Lipavský, K. Morawetz, and V. Špička,
Annales de Physique, Paris, 2001, No. 26, 1.

TT 71.69 Wed 15:00 Poster B

Electronic structure of substitutionally disordered systems: orbital based CPA within a pseudopotential approach — •Alexander Herbig, Rolf Heid, and Robert Eder — Institute for Solid State Physics, Karlsruhe Institute of Technology

Investigating the electronic structure of substitutionally disordered systems (e.g. doped compounds) is a challenge for density functional-based methods. A straightforward supercell approach is limited to special impurity concentrations due to its huge computational effort. In order to perform calculations at arbitrary impurity concentrations effective medium theories come into play. Among them the coherent potential approximation (CPA) has been successfully applied in the KKR-DFT-framework but rarely has been used within other DFT-frameworks. Blackman, Esterling and Berk (BEB) suggested an extension to the CPA which allows to handle off-diagonal disorder on the level of hopping-terms[1]. Based on ealier work[2], we developed a fully charge self-consistent BEB-CPA for a nonorthogonal LCAO-basis. This basis is obtained via projection from a mixed-basis pseudopotential calculation. We discuss the method itself as well as its numerical verification in comparison to model calculations for a tight binding binary alloy Hamiltonian solved by exact diagonalization. Furthermore we present first applications of the method to real materials.

[1] J.A. Blackman et al., Phys. Rev. B 4, 2412 (1971)
[2] K. Koerpenik et al., Phys. Rev. B 55, 5729 (1997)

TT 71.70 Wed 15:00 Poster B

Metal-Insulator Transition and Lattice Instability of Paramagnetic V_2O_3 — •I. Leonov[1], V. I. Anisimov[2,3], and D. Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Institute of Metal Physics, Yekaterinburg, Russia — [3]Ural Federal University, Yekaterinburg, Russia

We determine the electronic structure and phase stability of paramagnetic V_2O_3 at the Mott-Hubbard metal-insulator phase transition, by employing a combination of *ab initio* methods for calculating band structures with dynamical mean-field theory [1]. To explore structural transformations as a function of pressure, we use the experimentally determined atomic positions for the metallic and insulating phases, respectively, and calculate the total energy as a function of volume. We find that the structural stability depends very sensitively on changes of the lattice volume. The structural transformation associated with the metal-insulator transition is found to occur upon a slight expansion of the lattice volume by ~ 1.5 %, in agreement with experiment. Our results show that the structural change precedes the metal-insulator transition, implying a complex interplay between electronic and lattice degrees of freedom at the transition. Electronic correlations and full charge self-consistency are found to be crucial for a correct description of the properties of V_2O_3.

[1] I. Leonov, V. I. Anisimov, and D. Vollhardt, arXiv:1410.5399 (2014).

TT 71.71 Wed 15:00 Poster B

Investigating disorder effects in fabricating photonic quantum simulators on a kagome geometry: PEPS versus exact-diagonalization analysis — •Amin Hosseinkhani[1,2], Ali T. Rezakhani[3], and Hamed Saberi[4,5] — [1]Peter Grunberg Institute (PGI-2), Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany — [3]Department of Physics, Sharif University of Technology, Tehran 14588, Iran — [4]Department of Optics, Faculty of Science, Palacký University, 17. listopadu 12, 77146 Olomouc, Czech Republic — [5]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), University of Paderborn, D-33098 Paderborn, Germany

The energy spectra and photon transfer dynamics of a unit kagome cell is being explored by using a flexible numerical framework. A projected-entangled pair state (PEPS) ansatz to the many-photon wave function allows us to gain a detailed understanding of the effects of undesirable disorder in fabricating well-controlled and scalable photonic quantum simulators. The correlation functions associated with the propagation of two-photon excitations reveal intriguing interference patterns peculiar to the kagome geometry. Our results justify the use of the proposed PEPS technique for addressing the role of disorder in such quantum simulators and promises sophisticated numerical machinery for yet further explorations of the scalability of the resulting kagome arrays.

TT 71.72 Wed 15:00 Poster B

Calculating atomic multiplets across the periodic table — •Qian Zhang and Erik Koch — German Research School for Simulation Sciences, 52428 Jülich

The calculation of the multiplet structure of atoms with open shells requires two main ingredients: (i) realistic Coulomb matrix elements and (ii) the construction of states with well defined total angular momentum and spin. For the first we perform density functional calculations for isolated atoms or ions to determine the Slater-integrals of the electron-electron repulsion. For the second we use a simple ladder operator method to construct the multiplet states. We have implemented this approach in a web based application that allows the interactive calculation of multiplets for any atom/ion in the periodic table. In addition we can include the effects of spin-obit coupling. This allows us to compare the perturbative Russell-Saunders L-S and j-j coupling schemes to the more accurate intermediate coupling in which Coulomb repulsion and spin-orbit coupling are treated on the same footing.

TT 71.73 Wed 15:00 Poster B

Single-Particle Green's Function from the time-dependent Gutzwiller Approximation — •Konstantin Hobuss, Jörg Bünemann, and Florian Gebhard — Universität Marburg, Fachbereich Physik, Renthof 6, 35037 Marburg

We calculate the single-particle Green's function of the single-band Hubbard model from the time-dependent Gutzwiller Approximation within a Lagrange formalism [1]. In our approach, we add an electron with fixed wave vector $\vec{k}$ which can be interpreted as a small perturbation of the system. The Euler-Lagrange equations yield the dynamics of the corresponding variational parameters caused by the small perturbation. For the special case of a half-filled paramagnetic ground state, we find oscillations of the double occupancy with a frequency $\Omega^2 = 16\varepsilon_0^2\left(1-u^2\right)$ where $u = U/U_{\mathrm{BR}}$ is the interaction strength in terms of the Brinkman-Rice energy and ε_0 is the energy per site of the noninteracting system. From the dynamics of the variational parameters, we can compute the single-particle Green's function for all frequencies. At small excitation energies, we recover previous results for the Gutzwiller quasi-particle dispersion [2].

[1] J. Bünemann et. al., *New J. Phys.* **15** (2013), 053050.
[2] J. Bünemann et. al., *Phys. Rev. B* **67** (2003), 075103.

TT 71.74 Wed 15:00 Poster B

Configuration Path Integral Monte Carlo Simulations of the

Degenerate Homogeneous Electron Gas at Finite Temperatures — •Tim Schoof, Simon Groth, Jan Vorberger, and Michael Bonitz — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts Universität zu Kiel, Germany

Quantum Monte Carlo simulations of the homogeneous electron gas (HEG) in the highly degenerate regime are generally hampered by the Fermion sign problem [1]. However, accurate data for thermodynamic properties over a full range of densities at finite temperatures are of great interest for many systems, including warm dense matter, and for numerical modeling serving as input to finite-temperature DFT calculations [2]. The Configuration PIMC (CPIMC) method does not suffer from the Fermion sign problem in the non-interacting limit and allows for efficient ab-initio simulations of the HEG at high densities ($r_s \leq 1$) and low to moderate temperatures ($T/T_F \leq 1$) [3]. Comparisons of the method with approximate results from Montroll-Ward and higher order pertubation theory and Restricted PIMC calculations will be presented.

[1] E. W. Brown, B. K. Clark, J. L. DuBois, and D. M. Ceperley, Phys. Rev. Lett. 110, 146405 (2013).
[2] V. V. Karasiev, T. Sjostrom, J. Dufty, and S. B. Trickey, Phys. Rev. Lett. 112, 076403 (2014).
[3] T. Schoof, S. Groth, and M. Bonitz, Contrib. Plasma Phys. (2014), DOI: 10.1002/ctpp.20140072

TT 71.75 Wed 15:00 Poster B

Periodization in Cluster Dynamical Mean-Field Theory — •Malte Harland, Igor Krivenko, and Alexander Lichtenstein — Uni Hamburg, Hamburg, Germany

The Dynamical Mean Field Theory (DMFT) maps the lattice problem onto a single site coupled to an electron bath, i.e. the Mean Field. To include spatial correlations we use CDMFT, the cluster extension that connects a cluster of many correlated sites to an electron bath with a matrix-valued hybridization function. Whereas there is only one possible DMFT scheme for the single site, there are different schemes proposed for cluster calculations. They differ in the way they incorporate the lattice symmetry into the cluster calculation done by the impurity solver. We present a comparison of the self-energy and the cumulant periodization for different cluster sizes, applying it to a 1-dimensional chain as well as to the frustrated Kagome lattice. The CDMFT scheme we use is formulated in the real space. We solve the Hubbard cluster impurity model within a Hybridization Expansion Quantum Monte Carlo solver and compare the lattice Green's function and the local density of states to results of the Density Matrix Renormalization Group method.

TT 71.76 Wed 15:00 Poster B

Electronic correlations at the two-particle level: from bulk to the nanoscale — •Angelo Valli[1,2], Thomas Schäfer[2], Patrik Thunström[2], Georg Rohringer[2], Sabine Andergassen[3], Giorgio Sangiovanni[4], Karsten Held[2], and Alessandro Toschi[2] — [1]Democritos National Simulation Center, Consiglio Nazionale delle Ricerche, Istituto Of- ficina dei Materiali (IOM) and Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy — [2]Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria — [3]Institute for Theoretical Physics and CQ center for collective quantum phenomena, University of Tübingen, Tübingen, German — [4]Institute of Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany

We discuss the properties of local two-particle vertex functions within the framework of dynamical mean-field theory (DMFT). Their knowledge is required, e.g., to compute the local vertex corrections to dynamical response functions, and in order to include non-local spatial correlations within diagrammatic extensions of DMFT. Within the dynamical vertex approximation (DΓA) non-local spatial correlations can be generated by the (self-consistent) numerical solution of the parquet equations. This allows to treat fluctuations in all particle-hole and particle-particle scattering channels on equal footing, and to describe their interplay. As an application, we show how the information enclosed in the local vertex of DMFT can be exploited to *disentangle* the role of local and non-local correlations in Hubbard nano clusters.

TT 71.77 Wed 15:00 Poster B

Kinks and low-energy dynamics of correlated electron systems — •Markus Greger and Marcus Kollar — Theoretische Physik III, Zentrum für elektronische Korrelationen und Magnetismus, Universität Augsburg

We present a physical interpretation of kinks in the effective dispersion seen in angle-resolved photoemission spectroscopy (ARPES) within the framework of dynamical mean-field theory (DMFT). We relate the energy scale of kinks to the binding energy of the local quasiparticles, i.e., Kondo singlet. This interpretation of kinks provides a direct connection to an important intrinsic property of the quasiparticles in Fermi liquids. The Kondo singlet wavefunction is further characterized using the density matrix renormalization group (DMRG).

TT 71.78 Wed 15:00 Poster B

Development and Application of Full Configuration Interaction Quantum Monte Carlo Techniques for Strongly Correlated Electron Lattice Models — •Werner Dobrautz — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Applications of Quantum Monte Carlo techniques to strongly correlated electron lattice models, like the Hubbard model, are severely hindered by the existence of the renowned sign problem.

In diffusion Monte Carlo methods this problem can be avoided by imposing a certain nodal structure on the emerging ground state solution. This necessary prior knowledge is not needed in the recently developed Full Configuration Interaction Monte Carlo algorithm, but emerges during a simulation due to its formulation of particle dynamics in a fully anti-symmetrized space of Slater determinants. But the ensure convergence to the correct ground state a cancellation of positive and negative weighted particles on Slater determinants during simulation has to happen. But the required amount of simulated particles heavily depends on the chosen single-particle basis functions in which the Slater determinants are constructed.

The unitary group approach to the non-relativistic electron problem allows us to efficiently formulate the FCIQMC method in the space of eigenfunctions of the spin operator S. This not only greatly decreases the Hilbert space size of the problem, but also allows us to restrict solutions to specific total spin quantum numbers.

TT 71.79 Wed 15:00 Poster B

Non-local spin correlations in strongly interacting electron systems — •Friedrich Krien[1], Erik G. C. P. van Loon[2], Hartmut Hafermann[3], A.N. Rubtsov[4], and A.I. Lichtenstein[1] — [1]I. Institute of theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands — [3]Institut de Physique Theorique (IPhT), CEA, CNRS, 91191 Gif-sur-Yvette, France — [4]Department of Physics, Moscow State University, 119991 Moscow, Russia

We investigate a modified Hubbard model with non-local spin-spin coupling by means of EDMFT and the recently developed Dual Boson approach. Severe complications in the underlying impurity model are circumvented by coupling impurity spins only to spin waves along the z-axis. We develop and apply an approximation to optimally recover the impurity susceptibilities of the desired rotationally invariant system.

TT 71.80 Wed 15:00 Poster B

Spin-orbit coupling and its influence on the competing orders in the functional renormalization group method — •Mario Fink, Christian Platt, Werner Hanke, and Ronny Thomale — Institut für Theoretische Physik und Astrophysik Fakultät für Physik und Astronomie Am Hubland D - 97074 Würzburg, Germany

The effect of spin-orbit coupling plays an essential role in current research on topological insulators and topological superconductivity. To investigate the influence of spin-orbit coupling on the competing orders of quantum many-body systems, the functional renormalization group (FRG) seems to be one method of choice. We present an extended FRG method, which incorporates a spin-dependent formulation of the FRG flow equations. The unconventional superconductor Sr_2RuO_4 is considered one candidate system which exhibits an intricate interplay between spin-orbit interactions and competing many-body instabilities. In this context, our method is capable of testifying e.g. the symmetry and the origin of the superconducting gap on the α, β, and γ bands.

TT 72: Low-Dimensional Systems: Poster Session

Time: Wednesday 15:00–18:00 Location: Poster B

TT 72.1 Wed 15:00 Poster B

Detecting classical phase transitions using higher order Renyi entropies — •Wilfried Michel, Peter Broecker, and Simon Trebst — University of Cologne, Germany

Entanglement entropies have become a well-established tool to describe and characterize the ground-state properties of quantum many-body systems. In particular, these entropies allow to positively identify topological order and to detect and classify phase transitions even in the absence of any order parameter.

Though classical systems show no entanglement, one can define similar subsystem entropies that much like in the quantum case provide a generic way to study many features of classical systems. Here we consider so-called Renyi entropies, which are indexed by a positive integer $n \geq 1$ where the limiting case of $n = 1$ is the von-Neumann entropy.

In this contribution, we show how to efficiently calculate a series of higher-order Renyi entropies to high accuracy. This series of higher-order Renyi entropies is then used to calculate the classical analogue of the so-called entanglement spectrum using a maximum entropy approach. We illustrate this procedure for a number of classical models, including Ising and dimer models.

TT 72.2 Wed 15:00 Poster B

Phases and phase transitions in a rotated Kitaev model — •Eoin Quinn, Roderich Moessner, and Subhro Bhattacharjee — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

We investigate a variant of Kitaev's honeycomb model which also realises an exactly solvable quantum spin liquid, and analyse an extended phase diagram that takes into account Heisenberg perturbations and a magnetic field. The system has essential differences from the original construction of Kitaev, with interesting consequences appearing already in the exact solution. In an appropriate limit, the model reduces to a toric code model on a Kagome lattice. The effect of the Heisenberg interactions are examined using a combination of analytical and numerical approaches, and in the toric code limit we find a continuous quantum phase transition between the quantum spin liquid and a magnetically ordered phase which belongs to the 3D-XYxZ2 universality class.

TT 72.3 Wed 15:00 Poster B

Interplay of multiple charge-density-waves and superconductivity in $DyTe_3$ at high pressures — •Diego A. Zocco[1,4], Andreas Kapuvari[1], Aaron Sauer[1], Frank Weber[1], Parisiadis Paraskevas[2], Gaston Garbarino[2], Ian Fisher[3], James Hamlin[4], and Brian Maple[4] — [1]Institute for Solid State Physics, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany — [2]European Synchrotron Radiation Facility, F-38043 Grenoble Cedex, France — [3]Department of Applied Physics, Stanford University, CA 94305, USA — [4]Department of Physics, University of California, San Diego, CA 92093, USA

$DyTe_3$ is a quasi-two-dimensional system in which two successive incommensurate charge-density-wave (CDW) states appear upon cooling at ambient pressure ($T_{CDW,1} = 306\,K$, $T_{CDW,2} = 49\,K$). The suppression with pressure of the CDW order is followed by the emergence of superconductivity above 1 GPa and below 1.5 K, as shown by our measurements of electrical resistivity and ac-susceptibility. X-ray diffraction (XRD) experiments under pressure indicate that the lower CDW state merges with the upper one at an intermediate pressure, suggesting that the double-CDW state could be accessed directly below a single $T_{CDW}(P)$ line. The phase diagram obtained from XRD is compared with the results of our recent electrical resistivity experiments.

TT 72.4 Wed 15:00 Poster B

X-ray diffraction studies of charge-density-wave formation in $DyTe_3$ — •Aaron Sauer[1], Diego A. Zocco[1], Andreas Kapuvari[1], Frank Weber[1], Paula Giraldo-Gallo[2], Hsueh-Hui Kuo[2], and Ian R. Fisher[2] — [1]Institute for Solid State Physics, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany. — [2]Department of Applied Physics, Stanford University, CA 94305, USA.

We report measurements of the order parameters of the charge-density-wave (CDW) states in $DyTe_3$ using 4-circle x-ray diffraction from 5 K to 400 K. Rare-earth tritellurides (RTe_3) are quasi-two-dimensional materials in which CDW order develops in the Te-Te layers. The weakly-distorted tetragonal lattice allows, for the heavier rare-earth compounds, the formation of a second CDW state at lower temperatures, orthogonal to the first one. For example, $DyTe_3$ orders below $T_{CDW,1} = 306\,K$ and $T_{CDW,2} = 49$ K. The CDW order parameter is determined from the temperature evolution of the integrated intensity of the superstructure peaks. In particular, we studied how the upper CDW state is affected below $T_{CDW,2}$.

TT 72.5 Wed 15:00 Poster B

Superconductivity at the interface of $SrTiO_3$ and amorphous Al_2O_3 — •Roland Schäfer[1], Dirk Fuchs[1], Ahmed Sleem[1], Rudolf Schneider[1], Richard Thelen[2], and Hilbert von Löhneysen[1,3] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe — [2]Karlsruher Institut für Technologie, Institut für Mikrostrukturtechnik, 76021 Karlsruhe — [3]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe

We investigate the two-dimensional (2D) electron gas forming at the interface of TiO_2 terminated $SrTiO_3$ and amorphous Al_2O_3. The resistance drops on cooling from room temperature down to 200 mK in an usual way by a factor of up to 250. Below 200 mK the system becomes superconducting. We investigate the superconducting phase transition by analyzing voltage vs. current (V/I) characteristics as a function of temperature and magnetic field. The I/V characteristics show a power law scaling $V \propto I^{\alpha}$ at low bias with a temperature dependent exponent α which is close to 1 at high temperatures rises to 3 at around $T \approx 160$ mK and rapidly ascents on further lowering the temperature. This behaviour is typical for a Berezinskii-Kosterlitz-Thouless transistion found in 2D superconductive layers.

TT 72.6 Wed 15:00 Poster B

Superconducting fluctuations in systems with Rashba-spin-orbit coupling — •Stefan Beyl[1], Peter P. Orth[2], Mathias Scheurer[2], and Jörg Schmalian[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Deutschland — [2]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Deutschland

We investigate the BEC-BCS crossover in a two-dimensional system with Rashba-spin-orbit coupling. To include the effects of phase and amplitude fluctuations of the superconducting order parameter we perform a loop expansion of the effective field theory. We analyze in particular the probability of a low density superconducting quantum phase transition. The theory is relevant to $LaAlO_3/SrTiO_3$ interfaces and two-dimensional cold atom systems with synthetic gauge fields.

TT 72.7 Wed 15:00 Poster B

Oxygen stoichiometry of $LaTiO_3$ thin films studied by *in-situ* photoemission — •Philipp Scheiderer, Alex Goessmann, Michael Sing, and Ralph Claessen — Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), 97074 Würzburg, Germany

As in the famous oxide heterostructure $LaAlO_3/SrTiO_3$ (LAO/STO) a two dimensional electron system is found at the interface between the strongly correlated Mott insulator $LaTi^{3+}O_3$ and the band insulator STO. The stabilization of $LaTi^{3+}O_3$ requires strong reducing growth conditions since the thermodynamically stable bulk phase is the oxygen rich $La_2Ti^{4+}{}_2O_7$. Therefore, we have systematically studied the impact of the oxygen background atmosphere on $LaTi^{3+}O_3$ thin film growth by PLD. Reflection high-energy diffraction intensity oscillations of the specular spot indicate a layer by layer growth mode for thin films, which merges into the formation of islands for thicker films. *In-situ* photoemission measurements enables us to determine the oxidation state of Ti indicating excess or lack of oxygen present in the prepared samples. Our experiments show that even for films grown in vacuum, strong oxygen excess is present probably due to oxygen outdiffusion from the STO substrate. We find that an LAO buffer layer serves as an effective barrier for this process. The spectral weight of the lower Hubbard band, being a characteristic feature for the Mott insulating phase, is found to scale inversely with the amount of excess oxygen.

TT 72.8 Wed 15:00 Poster B

Resonant photoelectron spectroscopy of γ-Al_2O_3/$SrTiO_3$ heterostructures — •Philipp Schütz[1], Florian Pfaff[1], Michael Zapf[1], Judith Gabel[1], Lenart Dudy[1], Götz Berner[1], Yunzhong Chen[2], Nini Pryds[2], Victor Rogalev[3], Vladimir Strocov[3], Christoph Schlüter[4], Tien-Lin Lee[4], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Würzburg, Germany — [2]Department of Energy Conversion and Storage, Technical University of Denmark, Risø Campus, Denmark — [3]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland — [4]Diamond Light Source Ltd., Didcot, United Kingdom

The spinel/perovskite heterointerface between the band insulators γ-Al_2O_3 and $SrTiO_3$ hosts a two-dimensional electron system (2DES) with exceptionally high electron mobility. Soft x-ray resonant photoelectron spectroscopy at the Ti L absorption edge is used to probe the Ti 3d derived interface states. Marked differences in the resonance behavior are found for the $SrTiO_3$ valence band and the different interface states, which are observed in the band gap of $SrTiO_3$. A comparison to x-ray absorption spectra of Ti $3d^0$ and Ti $3d^1$ systems reveals the presence of different types of electronic states with Ti 3d character, i.e., oxygen vacancy induced, trapped in-gap states and itinerant states contributing to the 2DES. Furthermore, exposure to low doses of oxygen during irradiation allows for the controlled and reversible manipulation of the interfacial electronic structure, i.e., the in-gap state intensity and the valence band offset between $SrTiO_3$ and γ-Al_2O_3.

TT 72.9 Wed 15:00 Poster B

Synthesis and electrical transport properties of the $LaVO_3$/$SrTiO_3$ interface — •Richard Hentrich[1], Jens Hänisch[1,2], Ludwig Schultz[1], and Ruben Hühne[1] — [1]IFW Dresden, Germany — [2]ITEP, Karlsruhe Institute of Technology (KIT), Germany

We have investigated the two dimensional electron gas at the interface of band gap insulator $SrTiO_3$ and mott insulator $LaVO_3$ in comparison to the well-known, purely band insulating $LaAlO_3$/$SrTiO_3$ system. Thin films of $LaVO_3$ were grown epitaxially on TiO_2 terminated $SrTiO_3$ single crystal substrates using RHEED-monitored pulsed laser deposition. Optimal process parameters for layer-by-layer growth were found resulting in the growth of atomically smooth films of well-defined thickness. Electrical transport measurements revealed an insulator-metal transition at a film thickness of six unit cells, which is different to previously reported values. Conducting samples showed metallic behavior in a wide temperature range, with their conductivity showing little to no dependence on layer thickness. This led to the conclusion of the metallic behavior being a merely interface driven effect.

TT 72.10 Wed 15:00 Poster B

Torque magnetometry on two-dimensional electron systems at MgZnO/ZnO interfaces — •Schorsch Michael Sauther[1], Stephan Albert[1], Matthias Brasse[1], Joseph Falson[2], Yusuke Kozuka[2], Atsushi Tsukasaki[3], Marc Andreas Wilde[1], Masashi Kawasaki[2,4], and Dirk Grundler[1] — [1]Phys.-Dep. E10, TU München — [2]Dep. of App. Phys. and QPEC, University of Tokyo — [3]IMR, Tohoku University and JST PRESTO — [4]RIKEN CEMS

Two-dimensional electron systems (2DESs) in oxide heterostructures have created great interest in the recent years. We study the magnetization M of MgZnO/ZnO heterostructures with 2DESs of small carrier density and high mobility at low temperatures and in high magnetic fields B. We report the de Haas-van Alphen (dHvA) effect, non-equilibrium currents (NECs) and unexpected overshoots in $M(B)$. An investigation of the temperature dependence of the dHvA amplitude allows us to determine the effective masses of the electron systems. We find enhanced effective masses and enhanced dHvA amplitudes. The NEC signals are analyzed regarding their dependence on temperature and magnetic field sweep rate. We explain the unexpected overshoots of the dHvA amplitude by means of the magnetic thaw-down effect which allows us to identify the type and density of charged impurities in the heterostructures. In addition, we report a hysteretic feature in the dHvA effect that we discuss in the framework of quantum Hall ferromagnetism. The work is supported by the DFG via TRR80 and Grant-in-Aids for Scientific Research (S) No. 24226002 from MEXT, Japan, as well as by the Murata Science Foundation.

TT 72.11 Wed 15:00 Poster B

Temperature dependent optical spectra of magnetic excitations of a 4-leg ladder — •Ignacio Vergara[1], Kris Cöster[2], Luis Fels[1], Martin Valldor[1,3], Stefan Wessel[4], Kai Phillip Schimdt[2], and Markus Grüninger[1] — [1]II. Physicalisches Institut, Universität zu Köln — [2]Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund — [3]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Institut für Theoretische Festkörperphysik, JARA-FIT and JARA-HPC, RWTH Aachen University

In low-dimensional spin-1/2 cuprates, optical spectroscopy is a powerful tool for the study of magnetic excitations with total spin S=0, e.g., bimagnon-plus-phonon absorption. The simultaneous excitation of a symmetry-breaking phonon allows us to study the magnetic excitations at high energies ($\sim$ 0.1 - 1 eV) throughout the entire Brillouin zone, because the phonon takes care of momentum conservation. The line shape of the optical conductivity provides important information on the kinetics and on the interactions of the magnetic excitations.

Through n-leg S=1/2 cuprate ladders, one can explore the dimensional crossover between 1D and 2D systems. The magnetism of n-leg ladders is of particular interest due the possible relevance for high T_c superconductivity. We present temperature-dependent optical conductivity data of the 4-leg ladder $La_2Cu_2O_5$. We report on a pronounced two-triplon resonance and compare the results with optical spectra of a 2-leg ladder compound and theory (CUT, QMC). Calculations for open and closed boundary conditions give insight on the character of the observed excitations.

TT 72.12 Wed 15:00 Poster B

Mott metal-insulator transition induced by utilizing a glass-like structural ordering in low-dimensional molecular conductors — •Benedikt Hartmann[1], Jens Müller[1], and Takahiko Sasaki[2] — [1]Institute of Physics, Goethe-University Frankfurt, 60438 Frankfurt (M), Germany — [2]Institute for Materials Research, Tohoku University, Sendai, 980-8577, Japan

We utilize a glass-like structural transition in order to induce a Mott metal-insulator transition in the quasi-two-dimensional organic charge-transfer salt κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br. In this material, the terminal ethylene groups of the BEDT-TTF molecules can adopt two different structural orientations within the crystal structure, namely eclipsed (E) and staggered (S). When cooling through the glass transition at $T_g \simeq 75$ K, a small fraction that depends on the cooling rate remains frozen in the S configuration. We demonstrate that, when thermally coupled to a low-temperature heat bath, a pulsed heating current through the sample causes a very fast relaxation with cooling rates at T_g of order several 1000 K/min. The freezing of the structural orientation causes a decrease of the electronic bandwidth W with increasing cooling rate, and hence a Mott metal-insulator transition as the system crosses the critical ratio $(W/U)_c$ of bandwidth W to on-site Coulomb repulsion U. Due to the glassy character of the transition, the effect is persistent below T_g and can be reversibly repeated by melting the frozen configuration upon warming above T_g. A simple model allows for an estimate of the energy difference between the E and S state as well as the cooling rate dependent difference in population.

TT 72.13 Wed 15:00 Poster B

Thermal expansion and magnetostriction measurements of the mixed systems $Cs_2CuCl_{4-x}Br_x$ ($0 \leq x \leq 4$) — •Satya Krishna Thallapaka, Ulrich Tutsch, Lars Postulka, Bernd Wolf, Michael Lang, Natalia van Well, Franz Ritter, and Cornelius Krellner — Physics Institute, Goethe-University Frankfurt (M), SFB/TR 49, D-60438 Frankfurt (M), Germany

The mixed systems $Cs_2CuCl_{4-x}Br_x$ ($0 \leq x \leq 4$), including the two well-known end members Cs_2CuCl_4 and Cs_2CuBr_4, are classified as quasi-two-dimensional quantum antiferromagnets with different degrees of magnetic frustration. Due to a site-selective substitution of the halide atoms two distinct critical concentrations (x = 1 and x = 2) had been identified [1]. Especially the $Cs_2CuCl_2Br_2$ compound exhibits the potential to be the system with the highest degree of frustration within this series. We present low-temperature thermal expansion measurements down to 40 mK and magnetostriction experiments up to 14 T on the $Cs_2CuCl_2Br_2$ compound. While specific heat measurements reveal indications for magnetic order around 90 mK, no clear signatures were found in thermal expansion studies along the b axis. Here an in-T linear contribution was observed indicating a 1D character of the magnetic excitations. For fields above 5 T one finds a clear deviation from this linearity. These results are discussed with specific heat data and also compared with the thermodynamic properties of the pure Cs_2CuCl_4 compound.

[1] P. T. Cong et al., Phys. Rev. **B** 83, 064425 (2011)

TT 72.14 Wed 15:00 Poster B

Field-induced ordered phases in coupled spin-dimer systems — •L. Postulka[1], B. Wolf[1], U. Tutsch[1], M. Baumgarten[2], Y. Borozdina[2], D. Strassel[3], S. Eggert[3], and M. Lang[1] — [1]Physics Institute, Goethe-University, SFB/TR 49, D-60438 Frankfurt (M) — [2]Max-Planck-Institute for Polymer Research, SFB/TR 49, D-55128 Mainz — [3]Physics Department and Research Center OPTIMAS, University of Kaiserslautern, D-67663 Kaiserslautern

Materials built of antiferromagnetically-coupled S=1/2 dimers, allow to study finite-temperature critical phenomena under well-controlled conditions. Examples are the Bose-Einstein-condensation of magnons in 3D systems and Luttinger-liquid behaviour in 1D. In pure 2D materials one expects so-called topological order associated with the binding of vortices with opposite circulation as suggested by Berezinskii, Kosterlitz and Thouless. We present susceptibility data down to 27 mK of a newly synthesised S=1/2 spin dimer systems consisting of stable organic biradicals. The crystal structure suggests a 2D arrangement of the coupled dimers. We observe a field-induced ordered state characterized by a rounded double-peak structure. To obtain detailed information about the nature of the field-induced ordered phase we measured the temperature dependence of the susceptibility at the critical fields. These results are compared with quantum Monte Carlo simulations and measurements on a metal-organic compound, composed of layers of S=1/2 dimers, which lacks long-range 3D magnetic order down to at least 27 mK, but instead shows distinct 2D behaviour in its magnetic properties[1].

[1] Tutsch *et al.*, Nat. Commun. 5, 5169 (2014)

TT 72.15 Wed 15:00 Poster B

Field and angle dependent magnetoresistance oscillations in the normal and antiferromagnetic states of κ-(BETS)$_2$FeX$_4$ (X = Cl, Br) — •Michael Kunz[1], Ludwig Schaidhammer[1], Werner Biberacher[1], Natasha D. Kushch[2], and Mark V. Kartsovnik[1] — [1]Walther- Meißner-Institut, Garching, Germany — [2]Institute of Problems of Chemical Physics, Chernogolovka, Russia

The bifunctional materials κ-(BETS)$_2$FeX$_4$ (X = Cl, Br) are layered organic metals exhibiting both metallic and superconducting behaviour while carrying localised magnetic moments. These compounds show an anitferromagnetic ground state with Néel temperatures T_N of 0.46 K and 2.5 K respectively, while the electron system remains metallic even below T_N. Studies of field and angular sweeps of the interlayer magnetoresistance for different field directions revealed different kinds of angular-magnetoresistance-oscillations (AMRO) as well as Shubnikov-de Haas (SdH) oscillations. The experimental data will be discussed in the context of the Fermi surface properties and their response to the antiferromagnetic ordering.

TT 72.16 Wed 15:00 Poster B

Hints for a pressure-induced insulator-to-metal transition in low-dimensional CuNCN — •Estaline Amitha Francis[1], H. Rosner[2], and C. A. Kuntscher[1] — [1]Experimentalphysik 2, Universität Augsburg, D-86135 Augsburg, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

Copper oxide compounds show fascinating properties such as high temperature superconductivity, cooperative Jahn-Teller effect, spin-Peierls magnetic, and cooperative magnetic states. Copper carbodiimide (CuNCN) is the nitrogen-based analog of cupric oxide, where the oxygen anion O^{2-} is replaced with the isolobal carboiimide NCN^{2-}, resulting in a distorted octahedral with first-order Jahn-Teller effect. Infrared high-pressure measurements on CuNCN were performed over the frequency range 500–6000 cm^{-1} to probe the insulator-to-metal transition. The infrared phonons of CuNCN at 595 and 696 cm^{-1} show significant pressure-dependent softening. The phonon mode at 595 cm^{-1} shows a two-fold splitting at 5 GPa (P_{c1}) and further splittings around 11 GPa (P_{c2}). The absorption edge is observed around 1200 cm^{-1} for 0.3 GPa and shows a strong red shift above P_{c2}. Furthermore, we observe a smearing out of the phonon spectra above P_{c2}. The changes in the absorption edge and the smearing out of phonons are indications for a pressure-induced insulator-to-metal transition in CuNCN.

TT 72.17 Wed 15:00 Poster B

Ferromagnetic domains due to a double exchange mechanism — •Matthias Peschke and Michael Potthoff — I. Institut für Theoretische Physik, Hamburg, Deutschland

The doped one-dimensional Kondo lattice is known to be ferromagnetic for sufficiently strong exchange coupling J. Ferromagnetism is caused by a double-exchange mechanism, i.e., electrons gain kinetic energy for ferromagnetically aligned local moments. For one-dimensional ring structures, however, this seemingly clear situation becomes much more complicated. Employing Krylov-space methods for finite Kondo lattices at strong J, we find that a singlet ground state is favored in some cases depending on the electron number and the boundary conditions. We argue that, locally, the double exchange leads to ferromagnetic alignment but globally the local moments may form a domain structure to prevent ring processes of the electrons, which are unfavorable due to the Fermi statistics or due to the boundary conditions.

TT 72.18 Wed 15:00 Poster B

Calculation of correlation functions of the Heisenberg chain by means of a hidden fermionic structure — •Raphael Kleinemühl and Frank Göhmann — Bergische Universität Wuppertal

We study short-distance correlation functions of the homogeneous XXZ chain by means of a hidden fermionic structure discovered by Boos et.al. Using computer algebra we explicitly construct the fermionic operators needed in this approach. They act on the space of quasilocal operators on the XXZ chain. For small n we express products of local operators, like $\sigma_1^z\sigma_n^z$, in terms of the fermionic basis, i.e. by acting with creation operators on a certain vacuum state. Short distance correlation functions appear in various physical applications as e.g. in the calculation of moments of ESR spectral lines. Apart from that it is our goal to extend the approach in such a way that a calculation of correlation functions of large distances becomes possible.

TT 72.19 Wed 15:00 Poster B

Hardware-independent Parallelization of Matrix Product State Codes Using SciPAL — •Thomas Köhler[1], Johannes Hagemann[2], Salvatore R. Manmana[1], and Stephan C. Kramer[3] — [1]Institut f. Theoretische Physik, Universität Göttingen — [2]Institut f. Röntgenphysik, Universität Göttingen — [3]Max-Planck-Institut f. biophysikalische Chemie, Göttingen

The physical properties of low-dimensional, strongly-correlated quantum systems, as described by Hubbard-like or Heisenberg models, can efficiently be accessed by matrix product state (MPS) and density-matrix renormalization group (DMRG) methods. The key to an efficient MPS code is the optimization of the evaluation of concatenated matrix-matrix products for building the multi-particle states and an efficient compression of single-particle states by truncated singular value decompositions. Based on SciPAL's [1] expression templates for BLAS operations we have designed a domain-specific embedded language for computing the properties of MPS. Because SciPAL's expression templates are hardware-independent we can provide an objective comparison of the performance of CPU- or GPU-based computations and hybrid forms thereof.

[1] SciPAL: Expression Templates and Composition Closure Objects for High Performance Computational Physics with CUDA and OpenMP, S. C. Kramer and J. Hagemann, ACM TOPC (to appear).

TT 72.20 Wed 15:00 Poster B

Electronic Instabilities of the AA-Honeycomb Bilayer — •David Sánchez de la Peña[1], Michael Scherer[2], and Carsten Honerkamp[1] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52056 Aachen, Germany and JARA Fundamentals of Future Information Technologies — [2]Institute for Theoretical Physics, University of Heidelberg, D-69120 Heidelberg, Germany

We use a functional renormalization group approach to study the instabilities due to electron-electron interactions in a bilayer honeycomb lattice model with AA stacking, as it might be relevant for layered graphene with this structure. Starting with a tight-binding description for the four π-bands, modes of the dispersion are integrated out by successively lowering an infrared cutoff. For a given set of short-ranged interactions, the method allows for an unbiased investigation of the competing instabilities arising in the effective low-energy theory, and for the determination of the leading tendencies. The antiferromagnetic spin-density wave is an expected instability for dominant local repulsion among the electrons, but for nonlocal interaction terms also other instabilities occur. The resulting phase diagrams depending on the model parameters are presented. We compare our results to single-layer graphene and the more common AB-stacked bilayer, both qualitatively and quantitatively. Current prospects for the analysis of graphene systems using some of the latest developments in renormal-

ization group methods are also discussed.

TT 72.21 Wed 15:00 Poster B

Strongly Degenerate Fermions in 2D Quantum Dots at Finite Temperatures - Configuration Path Integral Monte Carlo — •Simon Groth, Tim Schoof, and Michael Bonitz — Institut for Theoretical and Astrophysics, Christian Albrechts Universität Kiel, Germany

Based on first principles, the configuration PIMC approach (CPIMC) allows for the exact computation of thermodynamic properties of strongly degenerate fermionic many-body systems with arbitrary pair-interaction [1,2]. Due to the fermion sign problem, this regime is not accessible with (standard) PIMC methods. Here, a Worm algorithm within the CPIMC formalism is presented which, in addition to standard thermodynamic observables, is capable of providing exact results for imaginary time correlation functions, i.e., in particular for the Matsubara Green function. The method is tested for a two-dimensional system of spin polarized, Coulomb interacting fermions in a harmonic trap. Further, sampling only paths from a subspace of the whole configuration space (Restricted CPIMC), the sign problem can be circumvented. The introduced systematic error vanishes with increasing degeneracy.

[1] T. Schoof, M. Bonitz, A. Filinov, D. Hochstuhl, and J. Dufty, Contrib. Plasma Phys. **51**, 687 (2011).

[2] T. Schoof, S. Groth and M. Bonitz, Introduction to Configuration Path Integral Monte Carlo, Chapter in: Complex Plasmas: Scientific Challenges and Technological Opportunities edited by M. Bonitz, K. Becker, J. Lopez and H. Thomsen (Springer 2014).

TT 73: Spincaloric Transport II (jointly with MA)

Time: Wednesday 15:00–17:00 Location: H 0110

TT 73.1 Wed 15:00 H 0110

Interface spin polarization in FM/Pt bilayers investigated by XRMR — •Christoph Klewe[1], Timo Kuschel[1], Jan-Michael Schmalhorst[1], Markus Meinert[1], Florian Bertram[2], Olga Schuckmann[3], Joachim Wollschläger[3], Matthias Opel[4], Francesco Della Coletta[4], Stephan Geprägs[4], and Günter Reiss[1] — [1]CSMD, Physics Department, Bielefeld University, Germany — [2]Division of Synchrotron Radiation Research, Lund University, Sweden — [3]Physics Department, Osnabrück University, Germany — [4]Walther-Meißner-Institut, BAdW, Garching, Germany

We demonstrate the suitability of x-ray resonant magnetic reflectivity (XRMR) for investigations of proximity induced interface spin polarizations. This technique was currently used to exclude magnetic proximity effects in $NiFe_2O_4$/Pt bilayers [1] in order to confirm the longitudinal spin Seebeck effect in this system, free from Nernst effects.

Here, we present photon energy dependent XRMR measurements (P09, PETRA III, DESY; ID12, ESRF) at the Pt L_3-absorption edge on Fe/Pt, and further investigations on the systems $Ni_{0.33}Fe_{0.66}$/Pt, $Ni_{80}Fe_{20}$/Pt, Ni/Pt, Fe_3O_4/Pt, and $Y_3Fe_5O_{12}$/Pt. A detailed analysis of the observed reflectivity curves based on varying magnetic profiles at the Pt interface and a comparison with ab initio calculations provides an accurate spatial distribution and quantitative values of the induced magnetic moments per Pt atom. We find a correlation of the Pt spin polarization and the Fe content of the adjacent ferromagnet, while we see no evidence for proximity effects in $Y_3Fe_5O_{12}$/Pt.

[1] T. Kuschel et al., submitted 2014, arxiv: 1411.0113

TT 73.2 Wed 15:15 H 0110

Bias-enhanced tunnel magneto-Seebeck effect in Co-Fe-B/MgO-based magnetic tunnel junctions — •Marvin von der Ehe[1], Alexander Boehnke[2], Marius Milnikel[1], Ulrike Martens[1], Vladyslav Zbarsky[1], Karsten Rott[2], Andy Thomas[2], Michael Czerner[3], Günter Reiss[2], Christian Heiliger[3], and Markus Münzenberg[1] — [1]Inst. f. Phys., Universität Greifswald, Germany — [2]CSMD, Physics Dep., Bielefeld University, Germany — [3]I. Phys. Inst., Universität Giessen, Germany

In recent spincaloritronic research, several groups have observed the tunnel magneto-Seebeck effect (TMS) in magnetic tunnel junctions (MTJs) incorporating CoFe electrodes and MgO tunnel barriers [1,2].

Here, we present an approach of tuning the TMS effect by applying a DC bias voltage to the MTJ while a temperature gradient is generated by laser heating. We prepared Co-Fe-B/MgO/Co-Fe-B magnetic tunnel junctions that show high TMR ratios and observed Seebeck voltages of several microvolt, generated locally in the MTJ layers. Our experiments show that the resulting thermocurrent can be tuned to exhibit an on/off- switching when the magnetization configuration of the electrodes is changed from parallel to antiparallel and vice versa. Consequently, very high bias-enhanced TMS ratios are obtained. This behavior can be understood by the interplay of the TMS effect and the ohmic properties of the MTJs for small voltages. Funding by DFG SPP 1538 is acknowledged.

[1] Walter, M., et al. Nature Mater. 10, 742 (2011)

[2] Liebing, N., et al. Phys. Rev. Lett. 107, 177201 (2011)

TT 73.3 Wed 15:30 H 0110

Magnonic spin currents in ferro- and antiferromagnetic materials — •Denise Hinzke, Severin Selzer, Ulrike Ritzmann, Frank Schlieckeiser, and Ulrich Nowak — Fachbereich Physik, Universität Konstanz, 78457 Konstanz

Recent experiments show that applied temperature gradients can excite magnonic spin currents in ferromagnetic (FM) materials [1]. These experiments have raised the question of the role of the relevant length scales for these spin currents. We perform atomistic spin model simulations using the Landau-Lifshitz-Gilbert equation to calculate these characteristic length scales of magnon propagation in the vicinity of temperatures gradients. Our numerical findings are supported by analytical descriptions [2]. Extending our investigations to antiferromagnetic (AFM) materials we determined the frequency dependent magnon propagation length and also simulate magnon propagation due to thermal excitation. One of our findings is that an applied temperature gradient can excite magnons still transporting heat even if the expected spin current is zero. Furthermore, it was shown that the maximisation of entropy drives FM domain walls (DW) in temperature gradients [3]. We extend our former numerical and analytical investigations of DW motion caused by magnon excitation to AFM materials and compare with FM materials [3]. We acknowledge financial support by the DFG through SFB 767 and through SPP "Spin Caloric Transport". [1] K. Uchida et al, Appl. Phys. Lett. 97, 122505 (2010) [2] U. Ritzmann et al. Phys. Rev. B 89, 024409 (2014) [3] D. Hinzke and U. Nowak, Phys. Rev. Lett. 107, 027205 (2011)

TT 73.4 Wed 15:45 H 0110

Spin-wave propagation through a magnonic crystal in a thermal gradient — •Thomas Langner, Andrii V. Chumak, Alexander A. Serga, Burkard Hillebrands, and Vitaliy I. Vasyuchka — Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, Erwin-Schrödinger-Str. 56, 67663 Kaiserslautern

Spin waves show a high potential to transport information in form of spin angular momentum. Magnonic crystals (MC), spin-wave waveguides with a periodic modulation of the magnetic properties, provide possibilities to code and process data in manifold ways. For the application of MC-based spin-wave devices it is of crucial importance to understand their behavior in thermally inhomogeneous surroundings since local heating might appear in real devices. We present studies on the dynamics of coherently excited spin waves in thermal gradients applied to a MC in form of an yttrium iron garnet (YIG) waveguide of varied thickness. We observe a broadening of the frequency bandgaps, the regions where spin-wave propagation is forbidden, as well as a decrease in the transmitted signal compared to the equilibrium temperature case. The mechanisms leading to these effects are discussed. The experimental results are accompanied by numerical calculations. A T-matrix formalism that includes the changes of the magnetic parameters induced by thermal gradients is used. We acknowledge financial support by the Deutsche Forschungsgemeinschaft (DFG) within priority program 1538 “Spin Caloric Transport“.

TT 73.5 Wed 16:00 H 0110

Magnetic field dependence of magnon accumulation in ferromagnets — •Ulrike Ritzmann, Denise Hinzke, and Ulrich

Nowak — Universität Konstanz, Konstanz, Germany

In the last years it was shown that in a magnetic material spin currents are created by applying temperature gradients. This spin currents are due to a net magnon current that propagates from the hotter towards to cooler region of the magnetic material [1].

We perform atomistic spin model simulation with the stochastic Landau-Lifshitz-Gilbert equation for different temperature profiles to study magnon accumulation and magnonic spin currents and its characteristic lengthscales in ferromagnetic insulators [2]. Furthermore, we present simulations regarding the magnetic field dependence of the magnon propagation in linear temperature gradients, which allow to control the excited spin current and tune the frequency spectra of the involved magnons. The results show an increasing signal with increasing length of the system with a saturating behavior in agreement with experimental measurements [3]. On the other hand, we study the magnetic field dependence of the magnon accumulation and find a decreasing accumulation for increasing magnetic field. Both effects can be explained with the frequency distribution of the propagating magnons that are excited in the temperature gradient and its dependence on the system parameters. We acknowledge financial support by the DFG through SFB 767 and through SPP "Spin Caloric Transport".

[1] K. Uchida et al., APL 97, 172505(2010); [2] Ritzmann et al., PRB 89, 024409 (2014); [3] Kehlberger et al., arXiv:1306.0784

TT 73.6 Wed 16:15 H 0110

Longitudinal spin Seebeck effect contribution in transverse spin Seebeck effect experiments in Pt/YIG and Pt/NFO — •Daniel Meier[1], Daniel Reinhardt[1], Michael van Straaten[1], Christoph Klewe[1], Matthias Althammer[2], Michael Schreier[2], Sebastian T. B. Goennenwein[2], Arunava Gupta[3], Maximilian Schmid[4], Christian H. Back[4], Jan-Michael Schmalhorst[1], Timo Kuschel[1], and Günter Reiss[1] — [1]CSMD, Physics Department, Bielefeld University, Germany — [2]Walther-Meißner-Institut, BAdW, Germany — [3]MINT Center, University of Alabama, USA — [4]Department of Physics, University of Regensburg, Germany

We investigated the inverse spin Hall voltage generated in a 10 nm thin Pt strip deposited on the magnetic insulators $Y_3Fe_5O_{12}$ (YIG) and $NiFe_2O_4$ (NFO) with a temperature gradient in the film plane. We observed characteristics typical of the spin Seebeck effect (SSE), although we did not observe a change of sign of the voltage at the Pt strip when the direction of the heat flow was reversed, which is believed to be the most striking feature of the *transverse* SSE. Therefore, we relate the observed signals to the *longitudinal* SSE generated by a parasitic out-of-plane temperature gradient, which can be simulated by contact tips of different material and heat conductivities and by tip heating [1]. This work [2] gives new insights into the interpretation of transverse spin Seebeck effect experiments, which are still under discussion.

[1] D. Meier et al., Phys. Rev. B 88, 184425 (2013)
[2] D. Meier et al., arXiv:1411.6790 (2014)

TT 73.7 Wed 16:30 H 0110

Thickness and temperature dependent thin film thermal conductance of YIG — •Christoph Euler[1], Paulina Holuj[1,2], Andreas Kehlberger[1,2], Mathias Kläui[1,2], and Gerhard Jakob[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität mainz, Staudinger Weg 7, 55128 Mainz — [2]Graduate School of Excellence 'Materials Science in Mainz', Staudinger Weg 8, 55128 Mainz

Thin film YIG ($Y_3Fe_5O_{12}$) is commonly used in spin-caloritronics, as it is a prototype material for experiments on thermally generated pure spin currents and the spin Seebeck effect. However, bulk values of the thermal conductance are often used to determine temperature gradients even if the actual experimental geometry employs thin films. The 3ω method is an established technique to measure the cross-plane thermal conductance of thin films, but it is inapplicable in YIG/GGG ($Ga_3Gd_5O_{12}$) systems in its standard form. We use two-dimensional modeling of heat transport and introduce a technique based on Bayesian statistics to evaluate measurement data obtained from the 3ω method. This allows us to extract the temperature dependent thermal conductance of thin film YIG between room temperature and 10 K even for films in the hundreds of nanometer thickness range, which are of major importance for experiments in the field of spin-caloritronics. Moreover, our developed generic data evaluation scheme is suitable to analyze all thin film 3ω measurements, which have so far not been accessible for analysis using the 3ω method. We gratefully acknowledge financial support by DFG (Ja821/7-1) and (GSC 266).

TT 73.8 Wed 16:45 H 0110

Optically-Reconfigurable Dynamic Magnetic Materials for the Control of Spin Waves — •Marc Vogel[1], Andrii V. Chumak[1], Erik H. Waller[1], Thomas Langner[1], Vitaliy I. Vasyuchka[1], Burkard Hillebrands[1], and Georg von Freymann[1,2] — [1]Department of Physics and State Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schroedinger-Str. 56, 67663 Kaiserslautern, Germany — [2]Fraunhofer-Institute for Physical Measurement Techniques IPM, Erwin-Schroedinger-Str. 56, 67663 Kaiserslautern, Germany

Spin waves - eigen excitations of the electrons' spin system - are of special importance nowadays due to the large potential for applications (e.g. processing, filtering or short-time storage of data). While all these applications rely on pre-defined constant structures, a dynamic variation of the structures opens access to novel physical phenomena and to novel applications. Here, we present the realization of such dynamic two-dimensional magnetic materials. By using laser light and a spatial light modulator, we reconstruct computer generated holograms on a ferrimagnetic yttrium iron garnet spin-wave waveguide. A black absorber (including carbon black nanoparticles) absorbs the light and creates thermal landscapes in the magnetic medium. The local change in temperature results in landscapes of the saturation magnetization. An acousto-optical modulator controls the temporal heating. Thus, the spin-wave characteristics can be controlled both in space and in time. The proposed fully-reconfigurable magnetic material is demonstrated using examples of one- and two-dimensional magnonic crystals.

TT 74: Focus Session: Ultra-Fast Magnetism under Electronic Nonequilibrium Conditions (organized by MA)

Organizers: U. Bovensiepen (U. Duisburg-Essen), Martin Eckstein (U. Hamburg), M. I. Katsnelson (U. Nijmegen)

Rapid control of magnetism is of high technological relevance for ultra-fast magnetic storage [Kirilyuk et al., RMP 82, 2731 (2010)]. Because the magnetic order emerges from electronic correlations, magnetism control can be pushed to the extreme time limit with ultra-short laser pulses that bring the electronic state out of equilibrium. For example, recent photoemission studies resolve the dynamics of the exchange splitting in ferromagnetic Gadolinium [Carley et al., PRL 109, 057401 (2012)], and photo-induced phase transitions are possible in materials with coupled orbital and spin order [Wall et al., PRL 103, 097402 (2009)]. When electrons are driven out of equilibrium, the magnetic exchange interaction itself can be manipulated by ultrafast carrier (photo) doping or by dressing the electronic states with light. On the theory side, recent developments like nonequilibrium dynamical mean-field theory [Aoki et al., RMP 86, 779 (2014)] allow to investigate electronic correlations in magnetically ordered systems out of equilibrum. This session will highlight recent experimental and theoretical developments which provide an understanding for the dynamics of magnetism in a regime where separation of slow spin and fast electron dynamics is no longer valid.

Time: Wednesday 15:00–17:45 Location: H 1012

Invited Talk TT 74.1 Wed 15:00 H 1012

Ultrafast optical tuning of ferromagnetism in EuO via the carrier density — •Manfred Fiebig — ETH Zürich, Department of Materials, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland

The interest in manipulating magnetic order by ultrashort laser pulses has thrived since it was observed that such pulses can be used to alter magnetization on a sub-picosecond timescale. In many cases demagnetization by laser heating dominates the dynamics; this is well described by the classic three-temperature model — assuming energy exchange between thermalized reservoirs of electrons, spins, and the lattice. Here we demonstrate a mechanism that allows the magnetic order of a material to be enhanced or attenuated at will. This is possible in systems simultaneously possessing a low, tunable density of conduction band carriers and a high density of magnetic moments. In such systems the thermalization time can be set such that adiabatic processes dominate the photoinduced change of the magnetic order — the three-temperature model is bypassed. In ferromagnetic $Eu_{1-x}Gd_xO$ we thereby demonstrate strengthening as well as weakening of the magnetic order by ∼10% and within ≤3 ps by optically controlling the magnetic exchange interaction. A theory backing up and expanding our experimental results will be presented.

Invited Talk TT 74.2 Wed 15:30 H 1012

Intra-atomic exchange in ultrafast magnetism — •Martin Weinelt — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany

The exchange interaction is the defining element in the formation of magnetic order in atoms and solids. Therefore the role of intra- and interatomic exchange during ultrafast magnetization dynamics needs to be explored. In the atomic magnetism of lanthanide metals localized $4f$ and itinerant $5d$ orbitals contribute to the overall magnetic moment. In general it is assumed that the intra-atomic exchange coupling is fast enough to be treated as an instantaneous process. We studied the magnetization dynamics of the lanthanide metals gadolinium [1] and terbium by time-resolved photoemission employing femtosecond higher-order harmonic vacuum-ultraviolet pulses. Recording in parallel $4f$ magnetic linear dichroism and $5d$ exchange splitting we observe distinct spin dynamics in Gd, which show the breakdown of the intra-atomic exchange upon femtosecond laser excitation. An orbital-resolved Heisenberg model [2] explains well the state-dependent two timescales of magnetization dynamics in Gd metal, which differ by one order of magnitude. Due to its much stronger spin-lattice coupling, Tb shows a distinctly different magnetization dynamics.

[1] Robert Carley *et al.*, Phys. Rev. Lett. **109** (2012) 057401.
[2] Soenke Wienholdt *et al.*, Phys. Rev. B **88** (2013) 020406(R).

15 min. break

Invited Talk TT 74.3 Wed 16:15 H 1012

Laser induced ultrafast demagnetization in solids: a time-dependent density functional theory perspective — •Sangeeta Sharma, J. K. Dewhurst, K. Krieger, P. Elliott, and E. K. U. Gross — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany.

Ultrafast manipulation of spins in a controlled manner is a milestone of solid state physics. The motivation for this is to use electronic spin for storing binary data, which can then be optically manipulated using lasers. Recent experiments have demonstrated that demagnetization or spin-reorientation processes can be induced by femtosecond laser pulses. However, we are still far from achieving optimally controlled manipulation of spins required for production of devices. One of the reasons behind this is the lack of full understanding of the phenomena leading to demagnetization.

Time-dependent density functional theory (TDDFT) is a formally exact method for describing the real-time dynamics of electrons under the influence of an external field – for example vector potential of the intense laser pulse. We use spin-resolved TDDFT to study of the process of optical demagnetization. The advantage of such a technique is clear from the fact that it is fully ab-initio in nature. Our analysis shows that the demagnetization occurs as a two step process where first the electrons make transitions to excited states, followed by spin-orbit-mediated spin-flip transitions which lead to a loss of moment. Non-collinearity of the spins does not play significant role in the demagnetization process.

Invited Talk TT 74.4 Wed 16:45 H 1012

Ultrafast control of the exchange interaction with electric fields — •Johan H. Mentink — Max Planck Research Department for Structural Dynamics, University of Hamburg-CFEL, 22761 Hamburg, Germany — Radboud University Nijmegen, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands

The strongest interaction between microscopic spins in magnetic materials is the exchange interaction J_{ex}. Therefore, ultrafast control of J_{ex} keeps the promise to control spins on ultimately fast timescales, potentially bypassing fundamental speed limits for the control of magnetism with magnetic fields. In this talk we provide theoretical evidence that the exchange interaction can be manipulated on ultrashort timescales by strong electric field pulses. Focusing on the prototype Mott-Hubbard insulator, we find very different effects for resonant and off-resonant photo-excitation. In the former case, the electron distribution is changed and the subsequent relaxation of photo-excited carriers causes an ultrafast reduction of J_{ex}. Conversely, off-resonant driving allows for an ultrafast and reversible control of J_{ex}, *i.e.*, it is active while the field is on, but leaves the electronic state unexcited after the pulse is switched off. In the regime of weak-driving strength the modification of J_{ex} is proportional to the intensity of the electric field and we find that J_{ex} can be enhanced and reduced for frequencies below and above gap, respectively. Furthermore, for strong driving even the sign of the exchange interaction can be reversed and we show that this causes time reversal of the associated quantum spin dynamics.

Invited Talk TT 74.5 Wed 17:15 H 1012

Controlling, probing and harnessing the strongest force in magnetism — •Alexey Kimel — Radboud University Nijmegen, Institute for Molecules and Materials, 6525 AJ Nijmegen, The Netherlands

The idea to change magnetic properties of media with the help of light has long intrigued people in physics and chemistry. Naturally, this raises the question about the speed limit of the optical control of magnetism. Fundamentally, magnetic order is a macroscopic manifestation of a quantum mechanical exchange coupling between spins. This exchange coupling represents the largest interaction in magnetism. It can be associated with an effective magnetic field of 100-1000 T. The strength can be appreciated from the fact that magnetic order in condensed matter survives well above room temperature. Obviously, harnessing the exchange interaction is the way to achieve the ultimately fastest magnetic switching. How can we control, probe and harness the exchange interaction for ultrafast magnetic switching? Here we demonstrate that the exchange interaction can be manipulated through ultrafast laser excitation in a large class of transition metal oxides. We show that using ultrashort laser pulses one can monitor laser-induced dynamics of the energy of the exchange interaction with subpicosecond temporal resolution. Finally, we suggest a scenario in which the strength of the exchange interaction is employed to achieve the fastest possible magnetic switching.

TT 75: Multiferroics II (jointly with DF, DS, KR, MA)

Time: Wednesday 15:00–18:50 Location: EB 107

Invited Talk TT 75.1 Wed 15:00 EB 107

Low energy consumption spintronics using multiferroic heterostructures — •Morgan Trassin — ETH Zurich, Zurich, Switzerland

Magnetization reversal in spintronics applications requires either an externally applied magnetic field or a large current density, which is accompanied by significant energy dissipation. A reversal of magnetization induced only by the application of an electric field would lead to low-power devices. Using multiferroics, previous approaches have seen limited success by only achieving rotations of the magnetization or a change in anisotropy by applying an electric field. To pave the way to new low-power devices, the more desirable electric-field driven magnetization reversal must be achieved and read out with a small current. In multiferroic heterostructures, ferromagnetic domains can be moved and switched using different charge states, strain configurations or magnetoelectric coupling. Ferroelectric domain engineering using epitaxial strain is critical towards the achievement of deterministic switchings. A combination of scanning probe microscopy and optical second harmonic generation were used to characterize multiferroic thin films strain state. Using electron microscopy and transport based techniques, a room temperature magnetization reversal of a CoFe thin layer solely induced by the application of a few volts to the heterostructure will be described.

TT 75.2 Wed 15:30 EB 107

Probing ferroic order in thin film heterostructures with optical second harmonic generation — •Gabriele De Luca, Manfred Fiebig, and Morgan Trassin — ETH Zurich, Switzerland

The evidence of the electric field control on the antiferromagnetic ordering in multiferroic bismuth ferrite ($BiFeO_3$) [1] increased interest in low energy consumption logic and memory devices. However, to exploit such functionality for devices it is essential to attain deterministic control of ferromagnetism at the single domain scale. Therefore a ferromagnet/multiferroic heterostructure has been designed based on the combination of magnetoelectric coupling in $BiFeO_3$ (BFO) and exchange coupling between magnetic materials thus offering a new pathway for the electrical control of magnetism [2,3]. Here we show that second harmonic generation (SHG), can detect the distribution of ferroelectric domains in BFO thin films non-invasively and unimpeded by transport properties. We use epitaxial strain for engineering different types of BFO domain patterns that are characterized by SHG, showing a unique relation between the domain distribution and the film symmetry. We then manipulate the BFO film by voltage poling and demonstrate the sensitivity of the SHG process to this manipulation. The concept applied to BFO is transferable to other multiferroics compounds thus indicating the general feasibility of SHG as a characterization technique for heterostructures in which buried ferroelectricity plays a key role in the emergence of magnetoelectric coupling. 1.Zhao et al., Nat. Mat. 5, 823 (2006) 2.Heron et al., Phys. Rev. Lett. 107, 217202 (2011) 3.Trassin et al., Phys. Rev. B 87, 134426 (2013)

TT 75.3 Wed 15:45 EB 107

Investigation of the antiferromagnetic coupling at $SrRuO_3$ / $La_{0.7}Sr_{0.3}MnO_3$ interfaces — •Sujit Das[1,2], Diana Rata[1], Andreas Herklotz[3], Er Jia Guo[4], Robert Roth[1], and Kathrin Dörr[1,2] — [1]Institute for Physics, MLU Halle-Wittenberg, 06099 Halle, Germany — [2]IFW Dresden, Postfach 270116, 01171 Dresden, Germany — [3]Oak Ridge National Lab., Oak Ridge, 37830 TN, USA — [4]Affiliation: Institute for Physics, Johannes-Gutenberg University Mainz, 55128 Mainz, Germany

$La_{0.7}Sr_{0.3}MnO_3/SrRuO_3$ superlattices grown on piezoelectric substrates show large antiferromagnetic coupling of the two ferromagnetic components and a significant strain effect on interfacial coupling [1]. Here we present a systematic investigation of the antiferromagnetic interface coupling in bilayers of $SrRuO_3$ (SRO) and $La_{0.7}Sr_{0.3}MnO_3$ (LSMO), grown by pulsed laser deposition (PLD) on (100)- oriented $SrTiO_3$ substrates. Epitaxial and coherent growth of the bilayers was confirmed by in-situ RHEED and ex-situ x-ray diffraction (XRD). Magnetic characterization was performed by SQUID magnetometry. We observed a strong dependence of the AFM coupling on the layer sequence and the thickness of the individual layers. The bilayers exhibit exchange bias, with the magnitude and sign of the exchange field strongly dependent on cooling field. Results of this study and ongoing work will be discussed. [1] Sujit Das et al, arXiv:1411.0411

TT 75.4 Wed 16:00 EB 107

Massive magnetoelectric modulation of the magnetic anisotropy in an epitaxial $La_{0.7}Sr_{0.3}MnO_3$/PMN-PT heterostructure — •Martin Wahler[1], Sujit Das[1], Kathrin Dörr[1], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

We use ferromagnetic resonance (FMR) to investigate the strain induced change of the in-plane magnetic anisotropy of an epitaxial ferromagnetic oxide layer on a piezoelectric substrate. The samples consist of 20 nm thick $La_{0.7}Sr_{0.3}MnO_3$ layers on two different substrates, namely $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$ (PMN-PT) (001) and (110) single crystals. The two substrates induce either isotropic or anisotropic in-plane strain, respectively. For $La_{0.7}Sr_{0.3}MnO_3$ on (001) PMN-PT substrate, it has already been demonstrated by SQUID magnetometry that the Curie-temperature and saturation magnetization can be changed by applying an electric field normal to the sample plane [1]. Here we show that for the same substrate orientation there is a small but significant change in FMR resonance fields along the directions of the magnetic easy axes. For the (110) substrate, however, a massive shift of the resonance fields is observed, resulting in a change of the uniaxial anisotropy of more than 0.5 kOe for an applied electric field of 12 kV cm^{-1}. All measurements are carried out at a temperature of 120 K.

[1] C. Thiele et al., Phys. Rev. B, **75** 054408 (2007)

TT 75.5 Wed 16:15 EB 107

Inverse TMR effect in multiferroic tunnel junctions studied from first principles — •Vladislav Borisov[1,2], Sergey Ostanin[2], and Ingrid Mertig[1,2] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg — [2]Max Planck Institute of Microstructure Physics

The spin-polarized electronic transport in multiferroic tunnel junctions (MTJ): Co/PTO/Co and LSMO/PTO/Co was computed from first principles. We confirm that the so-called four-state tunnelling magnetoresistance (TMR) may be detected for each MTJ when its TMR and TER are controlled by the reversible barrier polarization as well as reversible magnetization of the leads. The *ab initio* based results are directly compared to the experimental features of the inverse TMR recently reported for LSMO/PZT/Co [1]. We show how the observed effect originates from the magnetoelectric coupling seen at both interfaces of the MTJ [2]. The role of half-metallic LSMO as well as the effect of Zr substitutes in PTO are analysed in the context of the inversion of the TMR signal [1]. Another important issue of TMR discussed here concerns the functional (insulating) barrier thickness, which is always less than the nominal thickness and which depends on the polarization direction. We found that the functional barrier thickness is systematically reduced when the polarization is directed toward the Co electrode due to charge transfer at the Co/PTO interface.

[1] D. Pantel *et al.*, *Nat. Mater.* **11**, 289 (2012).
[2] V. S. Borisov *et al.*, *Phys. Rev. B* **89**, 054436 (2014).

TT 75.6 Wed 16:30 EB 107

Origin of superstructures in (double) perovskite thin films — •Vikas Shabadi, Marton Major, Philipp Komissinskiy, Aldin Radetinac, Mehran Vafaee, Wolfgang Donner, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Strasse 2, 64287 Darmstadt, Germany

We have investigated the origin of superstructure peaks as observed by X-ray diffraction of multiferroic $Bi(Fe_{0.5}Cr_{0.5})O_3$ thin films grown by pulsed laser deposition on single crystal $SrTiO_3$ substrates. The photon energy dependence of the contrast between the atomic scattering factors of Fe and Cr is used to rule out a chemically ordered double perovskite Bi_2FeCrO_6 (BFCO). Structural calculations suggest that the experimentally observed superstructure occurs due to unequal cation displacements along the pseudo-cubic [111] direction that mimic the unit cell of the chemically ordered compound [1]. This result helps to clarify discrepancies in the correlations of structural and magnetic

order reported for Bi_2FeCrO_6. The observation of a superstructure in itself is not a sufficient proof of chemical order in double perovskites.
[1] V. Shabadi, M. Major, P. Komissinskiy, M. Vafaee, A. Radetinac, M. Baghaie Yazdi, W. Donner, and L. Alff, J. Appl. Phys. **116**, 114901 (2014).

TT 75.7 Wed 16:45 EB 107

Using multiferroic systems as a spin filter - an ab initio study — •Stephan Borek[1], Jürgen Braun[1], Hubert Ebert[1], Angelika Chassé[2], Gerd Schönhense[3], Hans-Joachim Elmers[3], Dmytro Kutnyakhov[3], and Ján Minár[1,4] — [1]Ludwig-Maximilians-Universität München — [2]Martin-Luther-Universität Halle-Wittenberg — [3]Johannes-Gutenberg-Universität Mainz — [4]University of West Bohemia, Pilsen

Multiferroic heterostructures such as ultrathin Fe/$BaTiO_3$(001) films are of high interest for technical applications giving the opportunity to control the ferromagnetic state with an electric field or vice versa. In our theoretical study we investigated the effect of changing the electric polarization of the ferroelectric substrate $BaTiO_3$ on the ferromagnetic state of Fe and Co thin films using the method of Spin Polarized Low Energy Electron Diffraction (SPLEED). This method has been shown to be an effective tool for the investigation of surface properties like the determination of surface magnetic moments and the local crystal structure. The possibility of an application of the multiferroic heterostructures Fe/BTO(001) and Co/BTO(001) as a spin filter is discussed. It will be shown that a change of the polarisation of the $BaTiO_3$ results in a significant change of the exchange asymmetry giving the possibility to control the diffraction of electrons using the exchange interaction at the Fe (Co) surface. We focus on the systems of 1 ML, 2 ML and 3 ML Fe (Co) on $BaTiO_3$ because their electronic and magnetic structure as well as the coupling mechanism between the ferroic phases have been intensively discussed in the literature.

20 min coffee break

TT 75.8 Wed 17:20 EB 107

Optical investigation of ferroic domains beyond the resolution limit — •Christoph Wetli, Viktor Wegmayr, Thomas Lottermoser, and Manfred Fiebig — Department of Materials, ETH Zurich, Zurich, Switzerland

In recent years optical second harmonic generation (SHG) has been shown to be a versatile, non-destructive tool to investigate the often complex domain structures of ferroic and multiferroic materials. Ferroic domains vary broadly in structure and size, depending on the nature of the ferroic ordering. So far, however SHG was restricted to domains larger than the optical resolution limit of 1 μm. Here we present a method by applying a numerical model and simulation to overcome this limitation and to analyze ferroic domain structures some orders of magnitude smaller than the optical resolution limit. The method is based on the relation between the orientation of the ferroic order parameter and the phase of the nonlinear optical signal. It gives a relation between domain size and density, optical resolution and the intensity of the SHG signal. To show the reliability of the model, we applied it to several simulated domain structures. The simulation of the domain structures is based on an iterative geometrical algorithm, which allows us to generate complex domain patterns like the ferroelectric vortex structures or the irregular bubble like antiferromagnetic domains in hexagonal $YMnO_3$. The numerical calculations were compared with experimental data and found to be in excellent agreement.

TT 75.9 Wed 17:35 EB 107

Multiferroicity in $DyMnO_3$ thin films — •Chengliang Lu[1,2], Hakan Deniz[2], and Jun-Ming Liu[3] — [1]School of Physics, Huazhong University of Science and Technology, Wuhan 430074, China — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle(Saale), Germany — [3]Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China

The mutual control of ferroelectricity and magnetism is stepping towards practical applications proposed for quite a few promising devices in which multiferroic thin films are involved. Although ferroelectricity stemming from specific spiral spin ordering has been reported in highly distorted bulk perovskite manganites, the existence of magnetically induced ferroelectricity in the corresponding thin films remains an unresolved issue, which unfortunately halts this step. Here we report magnetically induced electric polarization and its gigantic response to magnetic field (an enhancement of 800% upon a field of 2 Tesla at 2 K) in $DyMnO_3$ thin films grown on Nb-$SrTiO_3$ substrates. Interestingly, we found a consecutive control of the polarization under a rotating magnetic field by detailed multiferroic response measurements. This is distinct to the standard polarization-flop process which results in a sudden change in polarization in multiferroics with spiral-spin-ordering state. The cooperative action of dual multiferroic mechanisms (the inverse Dzyaloshinskii-Moriya interaction among Mn moments and the exchange striction working between Dy and Mn moments) and phase coexistence associated with a twin-like structure was proposed as the origin of this phenomenon.

TT 75.10 Wed 17:50 EB 107

Observation of direct and converse local magnetoelectric switching at room-temperature in modified single-phase bismuth ferrite — •Leonard Frederic Henrichs[1], Oscar Cespedes[1], James Bennett[1], Joachim Landers[2], Wolfgang Kleemann[2], Heiko Wende[2], Doru Lupascu[2], and Andrew Bell[1] — [1]University of Leeds, Leeds, GB — [2]Universität Duisburg/Essen, Duisburd/Essen, Germany

Multiferroics are promising for applications in sensors and memory. However, no single-phase material with both ferroelectric and ferro- or ferrimagnetic order at room-temperature has been reported to date. Here, we observe very large local magnetoelectric coupling in the novel single-phase multiferroic $(BiFeCo_{0.1}O_3)_{0.4}$-$(K_{1/2}Bi_{1/2}TiO_3)_{0.6}$ at room-temperature. On ceramic samples, both direct and converse magnetoelectric switching was observed using piezoresponse force-microscopy and magnetic force-microscopy respectively. Areas where converse switching occurred, incorporate both a ferroelectric and magnetic domain-like cluster and thus appear to be (relaxor) ferroelectric and ferrimagnetic at room-temperature. The direct coupling-coefficient estimated from the experiments is 1.0×10^{-5} s/m, and thus extremely large. The locally observed converse meangetoelectric effect has a similar of magnitude. we propose that the material can be interpreted as a pseudo-nanocomposite with an ideal strain-mediated coupling due to congruent polar and magnetic nanoregions which are related to the relaxor ferroelectric and superparamagnetic nature of the material.

TT 75.11 Wed 18:05 EB 107

Tiny cause with large effects: the origin of the large magnetoelectric and magnetoelastic effect in $EuTiO_3$ — •Annette Bussmann-Holder — MPI-FKF, Heisenbergstr. 1, D-70569 Stuttgart, Germany

The magnetoelectric coupling in the perovskite $EuTiO_3$ is analyzed within a spin-phonon coupled Hamiltonian. It is shown that the tiny magnetostriction which accompanies the onset of antiferromagnetic order at $T_N = 5.7$ K induces a substantial hardening in the soft optic mode and a drop in the dielectric constant. The reduction of magnetostriction with increasing magnetic field reverses this behavior. While for small fields ferromagnetic order rapidly sets in accompanied by a volume expansion, this is destroyed with increasing fields and a strange paramagnetic state obtained. This exotic observation can be understood as stemming from the interplay between the enhanced oxygen p Ti d dynamical covalency which alters the crystal field at the Eu site and inhibits the virtual transition from $4f7$ to $4f65d$ responsible for ferromagnetic order.

TT 75.12 Wed 18:20 EB 107

First principles calculations on the effect of inner cationic site disorder, single and multiple cation and anion doping on the magnetic properties of $GaFeO_3$ — •Jacqueline Atanelov, Wernfried Mayr-Schmölzer, and Peter Mohn — Institute of Applied Physics - Computational Materials Science, Vienna University of Technology, Austria

$GaFeO_3$ is a promising multiferroic suitable for a wide range of applications in electronic devices. Motivated by that we investigate the influence of single and multiple cation and anion doping on the electronic and magnetic properties of gallium ferrite. Further we consider the well known fact of innner cation site disorder in $GaFeO_3$. In terms of cation doping we replace Ga atoms by Fe atoms and vice versa so that in total a concentration range of $0.9 \leq x \leq 2.0$ in $Ga_2 - xFe_xO_3$ is investigated. In addtion to that we substitute oxygen by B, C, N and S atoms. GFO is also known to show magnetic anisotropy for different cristallographic directions and sublattices. Beside changes in the total net magnetic moment induced by cation and anion doping, the magnetic anisotropy energy (MAE) can be affected as well. Doping

therefore can lead to an enhancement or reduction of the MAE. First principles density functional theory (DFT) calculations performed by the Vienna ab Initio Simulation Package (VASP) are used to predict and analyze the ground state electronic structure of the investigated systems.

TT 75.13 Wed 18:35 EB 107

Mechanism of interfacial magnetoelectric coupling in composite multiferroics — Chenglong Jia[1], Tongli Wei[1], Changjun Jiang[1], Desheng Xue[1], •Alexander Sukhov[2], and Jamal Berakdar[2] — [1]Key Laboratory for Magnetism and Magnetic Materials of MOE, Lanzhou University, Lanzhou 730000, China — [2]Institut für Physik, Martin-Luther-Universität, Halle-Wittenberg, 06099 Halle (Saale), Germany

We present a mechanism for the magnetoelectric coupling at ferroelectric/ferromagnetic interfaces based on screening via interfacial spin-rearrangement [1]. We find an electric-polarization-driven, non-collinear spin region extending over the spin-diffusion length in the ferromagnet. The orbital motion of the carriers in the ferromagnet is affected by the gauge field associated with the non-collinear spin order and hence indirectly by the electric polarization. Changing the latter, e.g., via an electric field influences the interfacial magnetic order and hence the spin-orbital coupled motion of the carriers. This allows for tuning the interfacial spin-dependent transport via electric fields. The resulting coupling is robust at room temperature and can be well approximated by a linear polarization- magnetization coupling, whose strength estimate for the composite Co(40 nm)/(tetragonal)$BaTiO_3$ is in line with recent experiments [2].

[1] C.-L. Jia, T.-L. Wei, C.-J. Jiang, D.-S. Xue, A. Sukhov, J. Berakdar, Phys. Rev. B **90**, 054423 (2014). [2] N. Jedrecy, H.J. von Bardeleben, V. Badjeck, D. Demaille, D. Stanescu, H. Magnan, A. Barbier, Phys. Rev. B **88**, 121409(R) (2013).

TT 76: Graphene: Applications, Luminescence, and Spin Relaxation (jointly with HL, O)

Time: Wednesday 16:45–18:45 Location: ER 270

TT 76.1 Wed 16:45 ER 270

Fabrication and Growth of Three-dimensional Graphene Electrodes with Controllable Pore Size — •Simon Drieschner, Michael Weber, Evangelos Makrygiannis, and Jose A. Garrido — Walter-Schottky-Institut, Physik Department, TU München, Am Coulombwall 4, 85748 Garching

Three-dimensional graphene-based electrodes combine graphene's unique properties like high conductivity, chemical inertness, and mechanical stability with a high surface to volume ratio, which could be of great interest for energy applications. However, tuning the pore size of 3D graphene networks is a non-trivial challenge, since the growth of graphene depends on the shape and structure of the metal substrate. Here we demonstrate the fabrication of 3D electrodes by using metal powder providing an interconnected scaffold which serves as substrate for the growth of graphene by chemical vapor deposition. The pore size distribution is shown to be controlled by the used metal particles and the growth temperature. After wet chemical etching of the metal catalyst, a freestanding and stable graphene foam of low mass and high crystalline crystal quality as confirmed by Raman spectroscopy is obtained. Cyclic voltammetry and electrochemical impedance spectroscopy measurements are used to confirm its excellent electrochemical properties. Our work highlights the great potential of these 3D graphene electrodes for energy storage and sensing applications.

TT 76.2 Wed 17:00 ER 270

Graphene microelectrode arrays for the electrochemical detection of neurotransmitters — •Martin Lottner[1], Luis Batista-Pires[2], and Jose A. Garrido[1] — [1]Walter Schottky Institut, TU München, München, Deutschland — [2]Catalan Institute of Nanoscience and Nanotechnology, ICN2, Barcelona, Spain

Graphene has great potential for use as stimulation and sensing material in neural and cardiac implants. Its flexibility and chemical stability anticipate a good biocompatibility, which cytotoxicity studies have underlined. It is transparent to visible light and non-magnetic, which allows for unperturbed optical stimulation and post-implantation MRT imaging. In this contribution, we present graphene microelectrode arrays for the electrochemical detection of neurotransmitters. Vacancy defects were introduced by ozone exposure and growth conditions were varied to increase double layer content of the electrodes. The modifications were validated using Raman spectroscopy. Cyclic voltammetry studies show an electrochemical window of about 1V. Ferricyanide redox studies have been performed upon increasing defect density and double layer content, to investigate the transition from macro- to microelectrode behaviour. Further, a sensitivity for the detection of norepinephrine and dopamine below 1nM is demonstrated. This study shows that modified CVD graphene microelectrodes can be used for highly sensitive detection of neurotransmitters. Taking advantage of the high interfacial capacitance and large electrochemical window of graphene electrodes, we will discuss their use for safe extracellular stimulation.

TT 76.3 Wed 17:15 ER 270

Structural study of mono- and bilayer graphene nanoribbons directly grown on SiC(0001) — •Lauren A. Galves, Timo Schumann, João Marcelo J. Lopes, and Henning Riechert — Paul-Drude-Institut für Festkorperelektronik, 10117 Berlin, Germany

Graphene nanoribbons (GNR) are very promising for nanoelectronics, since they possess unique electronic properties which are dependent on their width, edges, as well as number of graphene layers [1-2]. Therefore, achieving the controlled and high-quality synthesis of GNRs is anticipated to be of great importance. One of the methods which show great potential is the growth of GNRs on surface facets of SiC(0001) by the graphitization method [3]. In this contribution we report on the controlled growth and characterization of epitaxial mono- and bilayer GNRs on SiC(0001) surfaces. They were synthesized by utilizing the surface graphitization method at high temperatures and a straightforward air annealing (for bilayer GNRs) [4]. The influence of the surface step heights (i.e. facet sizes) on the ribbon growth and properties was analyzed. A correlation between steps heights and ribbons width was established. The nanostructures were analyzed by AFM height and phase contrast images. This allowed the determination of the SiC surface morphology as well as ribbons width. Raman spectroscopy was employed to gain information about the thickness of the GNRs (i.e. mono- or bilayer graphene) and their preferential edge type.

[1] V. Barone et al., Nano Lett. 6, 2748 (2006); [2] T.S. Li et al., Eur. Phys. J. 64, 73 (2008); [3] M. Sprinkle et al. Nat. Nanotechnol. 5, 727 (2010); [4] M.H. Oliveira Jr. et al., Carbon 52, 83 (2013).

TT 76.4 Wed 17:30 ER 270

Correlation of the crystallite sizes and D band frequency of non-graphitic carbons — •Dominique B. Schuepfer[1], Kristin Faber[2], Bernd M. Smarsly[2], Roman V. Yusupov[3], and Peter J. Klar[1] — [1]Institute of Experimental Physics I, Justus-Liebig-University Giessen, Germany — [2]Institute of Physical Chemistry, Justus-Liebig-University Giessen, Germany — [3]Institute of Physics, Kazan Federal University, Russia

Raman spectroscopy is often used to determine the crystallite size L_a of non-graphitic carbons by taking into account the intensity ratio of the defect-induced D band and the G band. We present an analysis of soft pitches via Raman spectroscopy in comparison to wide-angle X-ray spectra revealing discrepancies for L_a. Significant errors can be caused by known issues, for example the superposition of certain bands while estimating the intensities. Therefore, we introduce an alternative approach: An analysis of the D band revealed a correlation between its position and the crystallite size in the range of crystallite sizes less than 2 nm. The Raman shift significantly increases for smaller L_a using an excitation wavelength in the visible range. UV light yields the opposite behavior of the D band position, probably because of resonant absorption processes. To further characterize the samples in different L_a-ranges ($L_a < 2$ nm and $L_a > 2$ nm) electron paramagnetic resonance spectroscopy (EPR) has been carried out. Isotropic shaped EPR spectra are observed up to a crystallite size of 2 nm and samples containing crystallite sizes larger 2 nm show anisotropic signals. This behavior correlates with the detected Raman shift.

TT 76.5 Wed 17:45 ER 270

Ultrafast photocurrents in back-gated graphene — •Felix

Schade, Andreas Brenneis, Jose A. Garrido, Simon Drieschner, and Alexander W. Holleitner — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, Garching, Germany

We present picosecond time-resolved photocurrent measurements of back-gated CVD grown graphene on sapphire substrates. We examine the optoelectronic dynamics with respect to (i) the thermal coupling of graphene to its environment [1], (ii) different doping levels by tuning the back-gate voltage with respect to the Dirac point, and (iii) thermoelectric, photovoltaic as well as bolometric contributions. To this end, the graphene sheets are contacted by a THz-stripline circuit, and the ultrafast response is read-out by an Auston-switch [2]. The back-gate is separated from the graphene by the help of ALD-grown sapphire.

The ERC grant NanoREAL is acknowledged.

[1] A. Brenneis, et al., Nature Nanotechnology, DOI: 10.1038/NNANO.2014.276 (2015). [2] L. Prechtel, et al. Nature Comm. 3, 646 (2012).

TT 76.6 Wed 18:00 ER 270

Coherent and Incoherent Photoluminescene from Photo-excited Graphene — •Torben Winzer[1], Richard Ciesielski[2], Matthias Handloser[2], Alberto Comin[2], Achim Hartschuh[2], and Ermin Malic[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany — [2]Department Chemie, Ludwig Maximilians Universität München, Germany

Based on a microscopic theory and experimental measurements we investigate the ultrafast photoluminescence arsing from photo-excited graphene. Our calculations, performed within the density matrix formalism, allow for energy- and time-resolved insights into the radiative processes where two distinct microscopic mechanisms are distinguished: Beside the incoherent photoluminescence, which is driven by recombination of excited carriers, we find a coherent contribution induced by the microscopic polarization [1]. The incoherent spectrum mainly depends on the excitation strength. In contrast, the coherent photoluminescence spectrally shifts with the excitation energy, which is demonstrated for the first time and confirmed by our measurements.

[1] T. Winzer, R. Ciesielski, M. Handloser et al., arXiv:1411.0531v1 (2014)

TT 76.7 Wed 18:15 ER 270

Polarised Hot Carrier Photoluminescence in Graphene — •Thomas Danz, Andreas Neff, Reiner Bormann, Sascha Schäfer, and Claus Ropers — 4th Physical Institute, University of Göttingen, Göttingen, Germany

The thermalisation of photogenerated hot charge carriers in graphene leads to photoluminescence at wavelengths far away from that of the exciting pump laser [1,2]. To date, no polarisation properties of the photoluminescence have been reported, although recent numerical simulations show a strong anisotropy of the underlying relaxation processes in graphene [3]. This is in agreement with the results of transient pump-probe measurements showing a dependence of the transmissivity on the angle between pump and probe polarisations [4]. Here, we present polarisation- und time-resolved two-pulse excitation photoluminescence measurements with sub-30fs ultrashort laser pulses. We demonstrate an anisotropic nature of the emitted photoluminescence and use these findings to discuss complementary insights into the ultrafast carrier response in graphene.

[1] C. H. Lui *et al.*, Phys. Rev. Lett. **105**, 127404 (2010)
[2] W. Liu *et al.*, Phys. Rev. B. **82**, 081408 (2010)
[3] E. Malic *et al.*, Appl. Phys. Lett. **101**, 213110 (2012)
[4] M. Mittendorff *et al.*, Nano Lett. **14**, 1504 (2014)

TT 76.8 Wed 18:30 ER 270

Spin Relaxation in Graphene — •Frank Ortmann[1], Dinh. V. Tuan[2], David Soriano[2], Sergio O. Valenzuela[2,3], and Stephan Roche[2,3] — [1]Institute for Materials Science and Dresden Center for Computational Materials Science, TU Dresden, Germany — [2]ICN2 Barcelona, Spain — [3]ICREA, Barcelona, Spain

Spin polarization of electrons in graphene has been under great attention in recent years due to intrinsically small spin-orbit coupling and hyperfine interaction and high carrier mobilities. However, experimental spin-relaxation times are 3-4 orders of magnitude too short compared to theoretical predictions. Such discrepancy, together with contradictory proposals for spin-relaxation mechanisms, triggered a debate about its behavior in clean and/or defective graphene.

We observe an intrinsic spin-dephasing mechanism in graphene that is most strongly impacting the Dirac point, which can be enhanced by the adsorption of heavy ad-atoms.[1] The extracted spin relaxation times (τ_s) from our simulations show good agreement with experimentally observed energy dependencies of τ_s.

[1] D. V. Tuan, F. Ortmann et al. Nature Phys. 10, 857 (2014).

TT 77: Topological Insulators: Structure and Electronic Structure (jointly with HL, DS, MA, O)

Time: Wednesday 15:00–16:30 Location: ER 270

TT 77.1 Wed 15:00 ER 270

New electron states at the Bi/InAs(111) interface — K Hricovini[1,2], J-M Mariot[3], •L Nicolaï[1,2,7], U Djukic[1], M C Richter[1,2], O Heckmann[1,2], T Balasubramanian[4], M Leandersson[4], J Sadowski[4], J Denlinger[5], I Vobornik[6], J Braun[7], H Ebert[7], and J Minár[7,8] — [1]LPMS, UCP,Cergy, France — [2]DSM-IRAMIS, SPEC, CEA-Saclay, France — [3]LCP-MR, UPMC Univ. Paris 06/CNRS, France — [4]MAX-lab, Lund Univ., Sweden — [5]ALS, Berkeley, USA — [6]EST, Trieste, Italy — [7]LMU Münich, Germany — [8]Univ. of West Bohemia, Plzeň, Czech Republic

The Bi(111) surface is a prototype system to study Rashba-split surface states. Theoretical studies [1] predicted non-trivial topological surface states appearing on a single bi-layer of Bi(111) and a more complex behaviour was suggested for a variable film thickness as a function of layer thickness [2]. This clearly indicates that the electronic properties of thin films of this material are far from being understood. Here we present combined theoretical and ARPES studies of the electronic structure of Bi(111) films grown on InAs(111). Bi growth is epitaxial and a monocrystal of very high quality is obtained after depositing several monolayers. The ARPES experiments on these samples show several new types of electronic states. It is shown that a part of these new states corresponds to novel bulk-like features. These features are well reproduced by the one-step model of photoemission as implemented in the SPR-KKR package [3].[1] M. Wada et al., Phys. Rev. B 83, 121310 (2011). [2] Z. Liu et al., Phys. Rev. Lett. 107, 136805 (2011). [3] H. Ebert, D. Ködderitzsch, J. Minár, Rep. Prog. Phys. 74, 096501 (2011).

TT 77.2 Wed 15:15 ER 270

Ultrafast currents at the surface of the topological insulator Bi_2Se_3 — •Lukas Braun[1], Luca Perfetti[2], Gregor Mussler[3], Markus Münzenberg[4], Martin Wolf[1], and Tobias Kampfrath[1] — [1]Fritz-Haber-Institut Berlin (MPG) — [2]Ecole Polytechnique Palaiseau — [3]Forschungszentrum Jülich — [4]Universität Greifswald

Optical excitation of topological insulators (TIs) can launch electron currents along the TI surface whose direction can be controlled by varying the polarization of the driving light [J. W. McIver *et al.*, Nat. Nanotech. **7**, 96]. So far, photocurrents have been detected with a time resolution from DC to picoseconds [C. W. Luo *et al.*, Adv. Opt. Mat. **1**, 804]. Since electrons moving through a solid typically undergo scattering on a 100fs time scale, it is highly desirable to generate and detect TI photocurrents with femtosecond time resolution in a contact-free manner. For this purpose, we excite n-doped Bi_2Se_3 (Fermi energy at 300meV) crystals with a femtosecond laser pulse (10fs, 1.55eV). The resulting photocurrent gives rise to the emission of a broadband terahertz (THz) electromagnetic pulse (1 to 20THz) whose transient electric field is detected by means of electro-optic sampling. We present a method that allows us to extract the transient current $j(t)$ from the measured field $E(t)$. The AC photocurrents are found to be dominated by shift currents along the surface and photo-Dember injection currents into the bulk. We finally discuss the origin of $j(t)$ and implications for the dynamics of photoexcited TI electrons.

TT 77.3 Wed 15:30 ER 270

Observation of the photon drag effect in epitaxially grown $(Bi_{1-x}Sb_x)_2Te_3$ based topological insulators — •H. Plank[1], L. E. Golub[2], P. Olbrich[1], T. Herrmann[1], S. Bauer[1], V. V. Bel'kov[2], G. Mussler[3], J. Kampmeier[3], D. Grützmacher[3], and S. D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Jülich Aachen Research Alliance (JARA-FIT), Jülich, Germany

We report on the observation of a terahertz (THz) radiation induced photon drag effect in epitaxially grown $(Bi_{1-x}Sb_x)_2Te_3$ three-dimensional topological insulators. We demonstrate that the excitation with polarized radiation results in a dc electric photocurrent. While at normal incidence a current arises due to the photogalvanic effect in the surface states, caused by asymmetrical scattering of Dirac fermions [1], at oblique incidence it is overweighted by the trigonal photon drag effect. The currents are generated in n- and p-type $(Bi_{1-x}Sb_x)_2Te_3$ samples with various composition applying linearly and circularly polarized THz radiation. Results are analysed in terms of phenomenological theory and microscopic model based on transfer of photon momentum to free carriers resulting in an asymmetric distribution of electrons (holes) in k-space. Our analysis describes well all experimental findings including e.g. variation of the angle of incidence, radiation polarization and frequency. The observed trigonal photon drag and photogalvanic effect provide an opto-electronic method to study high frequency transport of Dirac fermions even at room temperature.

[1] P. Olbrich *et al.*, Phys. Rev. Lett. **113**, 096601(2014)

TT 77.4 Wed 15:45 ER 270

Cyclotron Resonance Induced Spin Polarized Photocurrents in Surface States of a 3D Topological Insulator — •K.-M. Dantscher[1], D.A. Kozlov[2], Z.D. Kvon[2], P. Faltermeier[1], M. Lindner[1], P. Olbrich[1], C. Zoth[1], G.V. Budkin[3], S.A. Tarasenko[3], V.V. Bel'kov[3], N.N. Mikhailov[2], S.A. Dvoretskii[2], D. Weiss[1], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Institute of Semiconductor Physics, Novosibirsk, Russia — [3]Ioffe Institute, St. Petersburg, Russia

We report on the observation of cyclotron resonance (CR) induced photocurrents excited by cw radiation, with frequencies of 2.54, 1.62 and 0.69 THz in a 3D topological insulator based on 80 nm strained HgTe films. To support the complex study, including optical, opto-electronic and electron transport experiments, various sample designs have been used. The measurements were done in a wide range of temperatures (1.6 to 120 K). We demonstrate that the photocurrent is generated in the topologically protected surface states. Studying the resonance response in the gated samples we examined the behaviour of the photocurrent and Dirac fermions cyclotron mass upon variation of Fermi energy. For large gate voltages we also detected CR in the bulk HgTe with the mass about two times larger than that obtained for the surface states. Based on this data we develop a microscopic theory of the effects and show that the asymmetry of light-matter coupling in the system of Dirac fermions subjected to an external magnetic field causes the electric current to flow. We show that the current is spin polarized.

TT 77.5 Wed 16:00 ER 270

Response of the topological surface state to surface disorder in $TlBiSe_2$ — Florian Pielmeier[1], •Andreas Eich[2], Gabriel Landolt[3,4], Bartosz Slomski[3,4], Julian Berwanger[1], Alexander A. Khajetoorians[5], Jens Wiebe[2], Roland Wiesendanger[2], Jürg Osterwalder[3], Franz J. Giessibl[1], and J. Hugo Dil[3,4,6] — [1]Institute of Experimental and Applied Physics, Universität Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany — [3]Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland — [4]Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [5]Institute of Molecules and Materials, Radboud University, 6500 GL Nijmegen, Netherlands — [6]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

By a combination of experimental techniques we show that the topmost layer of the topological insulator $TlBiSe_2$ as prepared by cleavage is formed by irregularly shaped Tl islands. No trivial surface states are observed in photoemission, which suggests that these islands can not be regarded as a clear surface termination. The topological surface state is, however, clearly resolved in photoemission experiments. This is interpreted as a direct evidence of its topological self-protection and shows the robust nature of the Dirac cone like surface state.

TT 77.6 Wed 16:15 ER 270

Wet etch process for HgTe nanostructure fabrication — •Kalle Bendias[1], Erwann Bocquillon[1], Alex Hughes[2], Christoph Brüne[1], Hartmut Buhmann[1], and Laurens W. Molenkamp[1] — [1]EP3, Physikalisches Institut, Universität Würzburg — [2]Department of Physics, Stanford University

Topological insulators (TI) are a new class of material with outstanding spin properties. Grown in 2d quantum wells HgTe does not only host Quantum Spin Hall edge channels [1][2], but also a giant Rashba splitting [3]. Both could lead to numerous applications in spintronic devices. In order to perform experiments such as spininjection, -probing [3] or quantum point contact collimation [4] a high carrier mobility and i.e. a long ballistic mean free path is essential.

The conventional processing method using ion milling to define the structure strongly affects these surface properties on small microstructures. In this talk the development and results of an alternative lithography etch method using KI:I:HBr as wet etchant are presented. Measurements on microstructures will be shown, indicating comparable mobilities on big and small structures.

[1] Markus König et al., Journal of the Physical Society of Japan 77.3 (2008), S. 031007.

[2] C. Brüne et al., Nature Physics 6.6 (2010), S. 448-454.

[3] J. Hinz et al., Semiconductor science and Technology 21.4 (2006), S 501-506.

[4] L.W. Molenkamp et al., Phys. Rev. B 41, 1274 (1990)

TT 78: Topological Insulators: Transport (jointly with HL, DS, MA, O)

Time: Wednesday 11:45–13:00 Location: ER 270

TT 78.1 Wed 11:45 ER 270

Surface Transport on a Bulk Topological Insulator — •Frederik Edler[1], Lisa Kühnemund[1], Marco Bianchi[2], Ellen M.J. Hedegaard[3], Martin Bremholm[3], Bo B. Iversen[3], Philip Hofmann[2], and Christoph Tegenkamp[1] — [1]Inst. f. Festkörperphysik, Uni. Hannover — [2]Dep. of Physics and Astronomy, Uni. Aarhus — [3]CMC, Dep. of Chemistry and iNANO, Uni. Aarhus

Topological insulators are guaranteed to support metallic surface states on an insulating bulk, and one should thus expect that the electronic transport in these materials is dominated by the surfaces states. Alas, due to the high remaining bulk conductivity, surface contributions to transport have mainly only been singled out indirectly via quantum oscillations, or for devices based on gated and doped topological insulator thin films, a situation in which the surface carrier mobility could be limited by defect and interface scattering. This issue was first overcome for Bi_2Te_2Se where compensation of defects leads to low bulk conductivity and surface-dominated transport could directly be observed [1]. Here we present a direct measurement of surface-dominated conduction on atomically clean surfaces of Bi_2Te_3. Using a four tip STM for nano-scale four point transport measurements with variable contact distance we show that the transport at 30 K is again two-dimensional rather than three-dimensional. The sheet conductivity is $7.9(3)\times10^{-4}\Omega^{-1}$ corresponding to a mobility of 505 cm^2/Vs. Besides, results regarding the temperature dependence of the conductivity and the influence of structural defects, e.g steps, present after cleavage will be discussed. [1] Barreto et al., Nano Lett. **14**, 3755 (2014)

TT 78.2 Wed 12:00 ER 270

Aharonov-Bohm oscillations in quantum wire of topological insulator — •Louis Veyrat[1], Joseph Dufouleur[1], Romain Giraud[1], Emmanouil Xypakis[2], Jens Bardarson[2], Christian Nowka[1], Silke Hampel[1], and Bernd Büchner[1] — [1]IFW-Dresden — [2]MPIPKS

Studying Aharonov-Bohm (AB) effect in a nanowire of topological insulator is a convenient way to reveal the specific properties of the topological surface states (SS), which are spin-chiral Dirac fermions. In the short perimeter limit, we evidenced in a previous work the ballistic transport of the SS in the perimeter of the nanowire, revealed by the temperature dependance of the phase coherence length [1] and showing the weak scattering effect of disorder on Dirac fermions. The quantum transverse confinement of SS is further revealed by the observation of non-universal conductance fluctuations. In the longer perimeter limit, we surprisingly find that the transport remains ballistic in the perimeter, despite the presence of disorder. The interaction with disorder is revealed by specific phase-jump of the AB oscillations under transverse magnetic field.

[1] Dufouleur et al., Phys. Rev. Lett. 110, 186806 (2013)

TT 78.3 Wed 12:15 ER 270

The effect of strain on the two-dimensional topological insulator HgTe — •Philipp Leubner, Andreas Budewitz, Christoph Brüne, Hartmut Buhmann, and Laurens Molenkamp — Experimentelle Physik III, Fakultät für Physik, Universität Würzburg, Germany

In the past years, HgTe quantum wells have been used extensively to study the magnetotransport signature of two-dimensional topological insulators, namely the quantum spin Hall effect. It has been shown that the band structure of those systems strongly depends on the thickness of the quantum well, and that, in particular, the topology changes from trivial to nontrivial at a critical thickness of 6.3 nm.

As an additional degree of freedom, the influence of strain on the band structure is investigated in this work. By using different CdTe-ZnTe superlattices grown on GaAs as virtual substrates, we are able to tune the strain of the HgTe quantum well layer from tensile to compressive, and thus modify the shape of the valence band.

Depending on strain, temperature dependent transport measurements on nominally identical wells reveal either features of topological insulators or semimetals, with the obtained fitting parameters nicely agreeing with band structure calculations. Further experiments focus on the correlation between the magnitude of the inverted bandgap and stability of the quantum spin Hall edge states.

TT 78.4 Wed 12:30 ER 270

Transport measurements on Mn-doped HgTe quantum wells — •Andreas Budewitz, Kalle Bendias, Philipp Leubner, Christoph Brüne, Hartmut Buhmann, and Laurens W. Molenkamp — Universität Würzburg, Lehrstuhl für experimentelle Physik III

In 2007 HgTe quantum wells have been experimental identified as a quantum spin Hall system [1]. One open question is how quantum spin Hall states interplay with magnetic impurities. Especially the formation of the anomalous quantum Hall effect raises a lot of interest [2, 3]. Since Mn-doped HgTe is a paramagnetic topological insulator it is important to investigate the onset of the $\nu = -1$ plateau at low fields. Here we present transport measurements on Mn-doped HgTe quantum wells. Therefore we show results on different temperatures, magnetic fields, Mn concentration and quantum well width. We discuss our results in comparison to undoped HgTe quantum wells.

[1] M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi and S.-C. Zhang, Science 318, 766 (2007)

[2] Chao-Xing Liu, Xiao-Lang Qi, Xi Dang, Zhong Fang and Shou-Cheng Zhang, PRL 101, 14682 (2008)

[3] Hsiu-Chang Hsu, Xin Liu and Chao-Xing Liu, Phys. Rev. B 88, 085315 (2013)

TT 78.5 Wed 12:45 ER 270

Quantum hall states equilibration in lateral heterojunctions on inverted HgTe quantum wells — •M. Reyes Calvo[1,2], Christoph Brüne[3], Christopher Ames[3], Philipp Leubner[3], Hartmut Buhmann[3], Laurens W. Molenkamp[3], and David Goldhaber-Gordon[1] — [1]Department of Physics, Stanford Universtiy, Stanford, U.S.A. — [2]C.I.C. Nanogune, San Sebastián, Spain — [3]Physikalisches Institut (EP3), Universität Würzburg, Würzburg, Germany

We study lateral heterojunctions on HgTe quantum wells with inverted band structure. At high densities and fields, we can explore the equilibration between Quantum Hall (QH) states with different filling factor. The resulting resistance plateaus are particularly clear in the n-n'-n quadrant and fit the expected values for a 2D electron gas heterojunction. The low density and moderate magnetic field regime is of more interest, since due to the inverted band structure of HgTe, Quantum Spin Hall (QSH) edge states could be present. In this regime, we observe unexpected features in the Hall resistance, which could be associated with the interplay between chiral QH edge modes and helical QSH edge modes.

TT 79: Frontiers of Electronic Structure Theory: Optical Excitation (organized by O)

Time: Wednesday 15:00–18:30 Location: MA 004

Invited Talk TT 79.1 Wed 15:00 MA 004

Ultrafast coherent dynamics in photovoltaics — •Carlo Andrea Rozzi[1], Sarah Maria Falke[2], Daniele Brida[3,4], Margherita Maiuri[4], Michele Amato[5], Ephraim Sommer[2], Antonietta De Sio[2], Angel Rubio[6,7], Giulio Cerullo[4], Elisa Molinari[1,8], and Christoph Lienau[2] — [1]CNR-NANO, Modena, Italy — [2]Carl von Ossietzky Universität, Oldenburg, Germany — [3]University of Konstanz, Germany — [4]CNR-IFN, Politecnico di Milano, Italy — [5]Universitè Paris-Sud, Orsay, France — [6]Universidad del País Vasco San Sebastián, Spain — [7]Fritz-Haber-Institut, Berlin, Germany — [8]Università di Modena e Reggio Emilia, Modena, Italy

The photoinduced charge-separation events occurring in photovoltaic systems have traditionally been interpreted in terms of the incoherent kinetics of optical excitations and of charge hopping, but recently signatures of quantum coherence were observed in energy transfer in photosynthetic bacteria and algae. We have studied charge separation in reference systems for artificial photosynthesis and photovoltaics by combining TDDFT simulations of the quantum dynamics and high time resolution femtosecond spectroscopy. We provide evidence that the coherent coupling between electronic and nuclear degrees of freedom is of key importance in triggering charge delocalization and transfer both in covalently bonded molecules and in bulk heterojunctions[1]. We have exploited the results of our research to design, syntesize and characterize a novel molecular scaffold for photovoltaic applications.[2]
[1] Falke S., et al., Science, 344, 1001 (2014) [2] Pittalis S., et al., Adv. Func. Mat. (2014)

TT 79.2 Wed 15:30 MA 004

Real-time propagation of coupled Maxwell-Kohn-Sham systems — •Rene Jestädt[1], Heiko Appel[1,3], and Angel Rubio[1,2,3] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain — [3]Max-Planck-Institut für Struktur und Materie, Hamburg

Based on a recent extension of time-dependent density-functional theory to quantum electrodynamics [1], we show first steps of an implementation of Maxwell's equations coupled to time-dependent Kohn-Sham equations. Our implementation utilizes the Riemann-Silberstein vector of the electromagnetic field which allows to write Maxwell's equations in a symplectic spinor representation similar to the Dirac equation. This spinor representation allows us to use standard unitary propagation techniques [2] developed for the Schrödinger equation also for the coupled solution of Maxwell's equations and Kohn-Sham equations. We illustrate our implementation of such coupled Maxwell-Kohn-Sham systems in the real-space real-time code octopus [3] for small molecules coupled to optical cavities [4].
[1] M. Ruggenthaler et al., Phys. Rev. A **90**, 012508 (2014).
[2] A. Castro et al., J. Chem. Phys. **121** (2004).
[3] X. Andrade et al., J. Phys. Cond. Mat. **24** (2012).
[4] M.S. Tame et al., Nature Physics 9, 329-340 (2013).

TT 79.3 Wed 15:45 MA 004

Correlated Light-Matter Interactions in Cavity QED — •Johannes Flick[1], Camilla Pellegrini[2], Michael Ruggenthaler[3], Heiko Appel[1,4], Ilya V. Tokatly[1,5], and Angel Rubio[1,2,4] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Nano-bio

Spectroscopy Group/ETSF Scientific Development Centre, Universidad del Pais Vasco UPV/EHU, San Sebastian — [3]Universität Innsbruck — [4]MPI for the Structure and Dynamics of Matter, Hamburg — [5]IKERBASQUE, Basque Foundation for Science, Bilbao

In the last decade, time-dependent density functional theory (TDDFT) has been successfully applied to a large variety of problems, such as calculations of absorption spectra, excitation energies, or dynamics in strong laser fields. Recently, we have generalized TDDFT to also describe electron-photon systems (QED-TDDFT) [1, 2]. Here, matter and light are treated on an equal quantized footing.
In this work, we present the first numerical calculations in the framework of QED-TDDFT. We show exact solutions for fully quantized prototype systems consisting of atoms or molecules placed in optical high-Q cavities and coupled to quantized electromagnetic modes. We focus on the electron-photon xc-contribution by calculating exact Kohn-Sham potentials using fixed-point inversions and present the performance of the first approximated xc-potential based on an optimized effective potential (OEP) approach.

[1] I. Tokatly, Phys. Rev. Lett. **110**, 233001 (2013).
[2] M. Ruggenthaler et.al., Phys. Rev. A **90**, 012508 (2014).

TT 79.4 Wed 16:00 MA 004

A hybrid QM/EMT approach to charge state corrections — •Osman Baris Malcioglu[1] and Michel Bockstedte[2] — [1]Lst.f.Theor.Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]FB Materialwissenschaften & Physik Universität Salzburg, 5020 Salzburg, Austria

Localized charge at surfaces, interfaces, or in volume materials naturally occur due to the ionization of adsorbates or defects. A robust quantitative description of charged systems is a prerequisite to explore the physics of adsorbates, surface and bulk defects of materials such as metal oxides. The popular supercell approach requires charge neutrality per supercell. For charged systems this is enforced by compensation charges. The resulting spurious interaction can be corrected a-posteriori [1,2]. Recently, a scheme based on model fitting the localized charge and dielectric screening was proposed [1]. Here, we present a fully automated and efficient hybrid QM/EMT approach for handling long-reach fields. The response of the medium and the localized charge density of the ab-initio calculations are represented by a finite element function space. The relevant physical observables are obtained using an auto-adaptive mesh solver. We demonstrate applications of our approach to charge state corrections of surface and bulk defects slabs in comparison with the earlier approaches [1,2].
[1] H.-P. Komsa and A. Pasquarello, Phys. Rev. Lett. **110**, 095505 (2013).
[2] C. Freysoldt, J. Neugebauer, and C. G. Van de Walle, Phys. Rev. Lett. **102**, 016402 (2009).

TT 79.5 Wed 16:15 MA 004

Plasmon assisted double photoemission — •Michael Schüler, Yaroslav Pavlyukh, and Jamal Berakdar — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

Coincidence measurements of double photoemission (DPE) represent a direct way of tracing the various facets of electronic correlations in molecular as well as extended systems, such as e. g. dynamical screening and collective excitations. One prominent example in this respect is the C_{60} molecule, for its plasmon resonances dominate the electronic excitation spectrum. Motivated by recent experiments on this molecule we demonstrate how the phenomenon of plasmon-mediated DPE can be described by an effective four-level system coupled to the bosonic plasmon excitations. The model generalizes the classical *s*-model and is treated within the *GW* approximation with the parameter estimates from *ab initio* calculations. We solve the coupled fermionic-bosonic time-dependent Kadanoff-Baym equations governing the dynamics of the model triggered by the interaction with the laser field. The use of the generalized Kadanoff-Baym Ansatz allows to significantly reduce the computation cost of our method.

TT 79.6 Wed 16:30 MA 004

Calculating photoemission spectra with real-time density-functional theory — •Matthias Dauth and Stephan Kümmel — University of Bayreuth, Germany

Photoemission spectroscopy is one of the primary tools for characterizing molecules and solids. A traditional approach of predicting photoemission signals relies on the interpretation of single-particle eigenvalues, e.g., from Hartree-Fock or Density Functional Theory (DFT). Here we demonstrate that real-time DFT allows for going beyond this static picture. We calculate photoemission signals dynamically and estimate ionization cross sections. We first investigate gas phase spectra, in which an ensemble of molecules with random orientation is probed. However, our approach in particular also allows for calculating angular resolved signals, i.e., we can track the ejected electron distribution with respect to a fixed light polarization. Furthermore, no a priori assumptions about the final state of the outgoing electrons need to be made, but the final state emerges naturally from the calculation. Thus, real-time DFT emerges as a powerful tool for the dynamical first-principles prediction of photoemission processes.

TT 79.7 Wed 16:45 MA 004

***Ab initio* local field effects for surface second harmonic generation** — •Nicolas Tancogne-Dejean[1,2] and Valérie Véniard[1,2] — [1]Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS-CEA/DSM, F. 91128, Palaiseau, France — [2]European Theoritical Spectroscopy Facility (ETSF), France

A comprehensive understanding of the nonlinear optical properties of solids is crucial to improve the design and the analysis of new optical devices. Among these processes, Second-Harmonic Generation (SHG) is probably one of the most studied and has become, through the years a very powerful-non-invasive technique to characterize materials, because of its particular sensitivity to the symmetry of a system. In materials where inversion symmetry is present, optical Second Harmonic Generation is forbidden within the dipole approximation. But at a surface or an interface between two such materials, the inversion symmetry is broken and SHG is allowed.

Crystal local fields are generated by the induced microscopic response of the system to an external perturbation. As a consequence their effects will be particularly important close to discontinuities as interfaces or surfaces. Local fields are important for a good description of optical properties of materials, but their effects on surface SHG have never been studied.

We present here a new ab initio formalism that allows us to calculate the frequency-dependent surface second-order susceptibility $\chi^{(2)S}$ within TDDFT, where the local field effects are fully included and we have applied this formalism to Silicon surfaces.

TT 79.8 Wed 17:00 MA 004

Mapping atomic orbitals in the transmission electron microscope: seeing defects in graphene — •Lorenzo Pardini[1], Stefan Löffler[2,3], Giulio Biddau[1], Ralf Hambach[4], Ute Kaiser[4], Claudia Draxl[1,5], and Peter Schattschneider[2,3] — [1]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [2]Institute of Solid State Physics, Vienna University of Technology, Austria — [3]University Service Centre for Transmission Electron Microscopy, Vienna University of Technology, Austria — [4]Central Facility for Electron Microscopy, University of Ulm, Germany — [5]European Theoretical Spectroscopy Facility (ETSF)

The possibility of mapping atomic orbitals by using energy-filtered transmission electron microscopy (EFTEM) has been considered for a long time and was recently demonstrated from a theoretical point of view. With the example of graphene, we predict how this approach can be used to map orbitals of a particular character. To this purpose, we have investigated graphene in its pristine structure and with two different kinds of defects, namely an isolated vacancy and a substitutional nitrogen atom. We show that basically three different kinds of images are to be expected, depending on the orbital character as determined from the corresponding projected density of states. To judge the feasibility of mapping such orbitals in a real microscope, we investigate the effect of the optics' aberrations, by simulating the lens system of two microscopes that are commonly used for electron energy loss spectrometry. We find that it should indeed be feasible to see atomic orbitals in a state-of-the-art EFTEM.

TT 79.9 Wed 17:15 MA 004

Inelastic X-Ray Scattering: Insights from and Benefits for Many-Body Theory — •Claudia Rödl, Igor Reshetnyak, Francesco Sottile, and Lucia Reining — Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau cedex, France

Non-resonant inelastic x-ray scattering (IXS) probes the momentum- and frequency-dependent dynamic structure factor $S(\mathbf{q}, \omega)$. It captures the neutral excitations of a many-body system, such as excitons, plasmons, and interband transitions. In particular, localized excitations that are forbidden in the optical limit of vanishing momentum trans-

fer are accessible. $S(\mathbf{q},\omega)$ is proportional to the diagonal element of the electric susceptibility $\chi(\mathbf{q},\mathbf{q}',\omega)$. Thus, IXS directly probes the dielectric screening and, hence, the screened Coulomb interaction which governs, for instance, the formation of quasiparticles in photoemission spectroscopy and excitons in optical spectroscopy. Therefore, IXS provides a unique tool to disentangle the many-body physics of renormalized quasiparticles and neutral excitations. It may serve as a solid experimental reference for the development of new approaches in many-body theory. Moreover, the off-diagonal elements of $\chi(\mathbf{q},\mathbf{q}',\omega)$ can be probed by coherent inelastic x-ray scattering (CIXS). This technique, which is still at a pioneering stage, allows one to visualize plasmon-like and localized neutral excitations in real space. We calculate diagonal and off-diagonal elements of $\chi(\mathbf{q},\mathbf{q}',\omega)$ for semiconductors and transition-metal oxides in good agreement with experiment and discuss the rich physics that is contained in $\chi(\mathbf{q},\mathbf{q}',\omega)$.

TT 79.10 Wed 17:30 MA 004

Real-Space Multiple-Scattering X-ray Absorption Spectroscopy Calculations of d- and f-state Materials using a Hubbard Model — •Christian Vorwerk[1], Kevin Jorissen[1], John Rehr[1], and Towfiq Ahmed[2] — [1]Department of Physics, University of Washington, Seattle, Washington 98195 USA — [2]Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545 USA

We present calculations of the electronic structure and x-ray spectra of materials with correlated d- and f-electron states treated with the Hubbard model in a real-space multiple scattering (RSMS) formalism, and using a rotationally invariant local density approximation (LDA+U). Values of the Hubbard parameter U are calculated ab initio using the constrained random-phase approximation (cRPA). The real-space Green's function approach with Hubbard model corrections is an efficient way to describe localized electron states in strongly correlated systems, and their effect on core-level x-ray spectra. The method is shown to give the correct density of states and x-ray absorption spectra for Transition Metal- and Lanthanide-oxides such as Ce2O3 and NiO, where the traditional RSMS calculations fail.

Supported by DOE BES DE-FG02-97ER45623

TT 79.11 Wed 17:45 MA 004

Variants of Second Order Screened Exchange for spin polarized and non-polarized Uniform Electron Gas — •Felix Hummel and Georg Kresse — University of Vienna, Austria

The commonly used Random Phase Approximation (RPA) only contains exchange processes of first order. The Second Order Screened Exchange (SOSEX) correction includes one exchange process beyond first order, which is considered the leading order correction to the RPA, and it has proven to be very accurate for the Uniform Electron Gas (UEG) as well as for solids.

The memory requirement of SOSEX is however of $O(N^4)$. We present an approach with a memory requirement of $O(N^2)$ and its differences to other approaches with comparable complexity, such as AC-SOSEX, for the spin polarized and non-polarized UEG.

TT 79.12 Wed 18:00 MA 004

Ferromagnetism from strongly correlated electrons at the $LaAlO_3/SrTiO_3$ interface — •Frank Lechermann, Lewin Boehnke, Malte Behrmann, Daniel Grieger, and Christoph Piefke — I. Institut für Theoretische Physik, Universität Hamburg

We shed light on the interplay between structure and many-body effects relevant for itinerant ferromagnetism in $LaAlO_3/SrTiO_3$ heterostructures. The realistic correlated electronic structure is studied by means of the (spin-polarized) charge self-consistent combination of density functional theory (DFT) with dynamical mean-field theory (DMFT) beyond the realm of static correlation effects [1]. A ferromagnetic instability occurs only with oxygen vacancies and it is possible to account for the basic mechanism by an derived minimal Ti two-orbital e_g−t_{2g} description for the correlated subspace. Magnetic order affected by quantum fluctuations with a Ti moment of $0.2\mu_B$ builds up from effective double exchange, which can be traced to the dilute defect regime. [1] F. Lechermann, L. Boehnke, D. Grieger and C. Piefke, Phys. Rev. B 90, 085125 (2014)

TT 79.13 Wed 18:15 MA 004

NanoDMFT: Full ab initio description of strong correlations in nanoscale devices — •David Jacob — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

In order to obtain a full first-principles description of the correlated electronic structure and transport properties of nanoscale devices we combine the Coulomb-Hole-Screened-Exchange (COHSEX) approximation with Dynamical Mean-Field Theory (DMFT). While the former yields an effective mean-field description of the weakly correlated conduction electrons, the DMFT part accounts for the dynamic correlations originating e.g. from the strongly interacting $3d$- or $4f$-shells of transition metal atoms or from the molecular orbitals of weakly coupled molecular devices. The combination with COHSEX instead of Density Functional Theory (DFT) improves upon our NanoDMFT approach [1] in two important aspects: First, from the screened interaction W we can calculate the effective Coulomb interaction U for the strongly interacting electrons. Second, unlike in DFT+DMFT calculations the double-counting correction for COHSEX+DMFT is exactly known and straight-forward to calculate. Hence the two quantities which are essentially parameters in the DFT based approach can now be calculated ab initio so that it is now possible to actually predict e.g. the occurance of the Kondo effect in magnetic atoms and molecules on metal surfaces and attached to metallic leads.

[1] D. Jacob *et al.*, PRL **103**, 016803 (2009); D. Jacob *et al.*, PRB **82**, 195115 (2010); M. Karolak *et al.*, PRL **107**, 146604 (2011); D. Jacob *et al.*, PRB **88**, 134417 (2013)

TT 80: 2D Materials Beyond Graphene: TMDCs, Silicene and Relatives (organized by O)

Time: Wednesday 15:00–17:45 Location: MA 005

TT 80.1 Wed 15:00 MA 005

Imaging spin-valley-layer locking in a transition-metal dichalcogenide — J.-M. Riley[1], F. Mazzola[2], M. Dendzik[3], M. Michiardi[3], T. Takayama[4], L. Bawden[1], C. Granerød[2], M. Leandersson[5], T. Balasubramanian[5], M. Hoesch[6], T. Kim[6], H. Takagi[4], W. Meevasana[7], Ph. Hofmann[3], M.-S. Bahramy[8], J.-W. Wells[2], and •Phil D.C. King[1] — [1]SUPA, University of St. Andrews, UK — [2]Norwegian University of Science and Technology, Norway — [3]Aarhus University, Denmark — [4]Max Planck Institute for Solid State Research, Germany — [5]MAX IV Laboratory, Sweden — [6]Diamond Light Source, UK — [7]Suranaree University of Technology, Thailand — [8]University of Tokyo, Japan

A strong locking between the spin and the valley pseudospin in monolayer transition-metal dichalcogenides (TMDCs) such as MoS_2 and WSe_2 opens unique potential for their use in novel quantum devices exploiting the valley degree of freedom. Here, using spin- and angle-resolved photoemission spectroscopy, we show that such spin-valley coupling persists in bulk 2H-WSe_2 where it becomes further entangled with the layer pseudospin [1]. Enormous spin splittings up to $\sim$0.5 eV result, despite the centrosymmetric nature of the bulk structure which would conventionally preclude the presence of spin polarised states. We argue these occur here due to local inversion symmetry breaking within constituent sub-units of the bulk unit cell, leading to a spin texture that is strongly modulated in both real and momentum space, and allowing us to directly image TMDC spin-valley-layer locking for the first time. [1] Riley *et al.*, Nature Phys. **10** (2014) 835.

TT 80.2 Wed 15:15 MA 005

From optics to superconductivity: Many body effects in transition metal dichalcogenides — Malte Rösner[1,2], Gunnar Schönhoff[1,2], Alexander Steinhoff[1], Frank Jahnke[1], Christopher Gies[1], Stephan Haas[3], and •Tim Wehling[1,2] — [1]Institute for Theoretical Physics, University of Bremen, D-28359 Bremen, Germany — [2]Bremen Center for Computational Material Sciences, University of Bremen, D-28359 Bremen, Germany — [3]Department of Physics and Astronomy, University of Southern California, Los Angeles, CA 90089-0484, USA

We discuss many body effects in MoS_2 ranging from optical properties to the emergence superconductivity (SC) and charge density wave phases (CDW). Combining ab-initio theory and semiconductor Bloch equations we show that excited carriers cause a redshift of the exci-

tonic ground-state absorption line, while higher excitonic lines disappear successively due to a huge Coulomb-induced band gap shrinkage of more than 500 meV and concomitant exciton binding-energy reductions. Upon strong charge doping, we observe a succession of semiconducting, metallic, SC, and CDW regimes. Both, the SC and the CDW instabilities trace back to a Kohn anomaly and related softening of Brillouin zone boundary phonons.

Invited Talk TT 80.3 Wed 15:30 MA 005

2D silcon materials: From single layer silicene to double-layer structures and multi-layer stacks — •Patrick Vogt — Institut für Festkörperphysik,Technische Universität Berlin, Deutschland

Silicene, a new silicon allotrope with a graphene-like honeycomb structure, has attracted considerable interest, because its topology confers to it the same remarkable electronic properties as those of graphene [1]. Additionally, silicene might have a potential advantage of being easily integrated in current Si-based nano/micro-electronics offering novel technological applications. However, silicene does not exist in nature and had to be synthesized on a substrate material [2].

We will describe the recent development on the epitaxial formation of single layer silicene on Ag(111), including structural and electronic properties. Based on these results we will look at the growth of silicene double-layer and multi-layer structures and discuss if they can be explained by the stacking of single silicene sheets [3]. If confirmed, such multi-layer structures could open the way towards the technological applicability of silicene.

[1] G.G. Guzmán-Verri, L.C. Lew Yan Voon, Phys. Rev. B 76, 075131 (2007); S. Lebègue and O. Eriksson, Phys. Rev. B, 79 115409 (2009); S. Cahangirov et al., Phys. Rev. Lett. 102, 236804 (2009).

[2] P. Vogt et al., Phys. Rev. Lett. 108, 55501 (2012); C.-L. Lin et al., Appl. Phys. Exp. 5, 045802 (2012); B. Feng et al., Nano Lett. 11, 3507 (2012); A. Fleurence et al., Phys. Rev. Lett. 108, 245501 (2012).

[3] P. Vogt et al., Appl. Phys. Lett. 104, 021602(2014), De Padova et al., Appl. Phys. Lett. 102, 163106 (2013)

TT 80.4 Wed 16:00 MA 005

The electronic band structure of MoS_2 investigated by ARPES — •Mathias Gehlmann[1], Sven Döring[1], Markus Eschbach[1], Ewa Mlynczak[1], Irene Aguilera[2], Gustav Bihlmayer[2], Stefan Blügel[2], Lukasz Plucinski[1], and Claus M. Schneider[1] — [1]PGI-6, FZ-Jülich — [2]PGI-1/IAS-1, FZ-Jülich

MoS_2 belongs to transition metal dichalcogenides and has drawn a large amount of attention in recent years. While the main area of interest in this material lies in the possibility of integrating it into two dimensional semiconductors and transistor devices, a growing number of researchers focuses on the valley polarization at the edge of the Brillouin zone.

We combine angle-resolved photoemission spectroscopy (ARPES) with density functional theory calculations to perform a thorough analysis of the valence band electronic structure of MoS_2. Our focus lies on the splitting of the valence band around the K point at the edge of the Brilluin zone, and on the comparison of the electronic states of the bulk material and its surface to a free standing monolayer.

TT 80.5 Wed 16:15 MA 005

Photocurrent studies on semiconducting MoS_2 — •Anna Vernickel[1,2], Marina Hoheneder[1,2], Eric Parzinger[1,2], Alexander Holleitner[1,2], and Ursula Wurstbauer[1,2] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 München, Germany

Atomically thin molybdenum disulfide (MoS_2) has gained increasing interest as very promising material for novel and innovative device applications. Its bandgap in the visible range and the transition to a direct semiconductor in the single-layer case make MoS_2 particularly suitable for optoelectronic devices. We report on extensive photocurrent spectroscopy studies of single and few-layer MoS_2 in order to investigate their optoelectronic properties. We discuss the impact of Schottky contacts and thermoelectric contributions to the observed photocurrent. To further investigate the underlying photocurrent dynamics, nanoscale electronic circuits facilitating access to the photocurrent evolution on a picosecond time scale are prepared. We gratefully acknowledge financial support by NIM and BaCaTec.

TT 80.6 Wed 16:30 MA 005

Hot electron dynamics at $2H$-MoS_2 surfaces: Time- and angle-resolved photoelectron spectroscopy results — •Petra Hein, Ankatrin Stange, Kerstin Hanff, Gerald Rohde, Michael Bauer, and Kai Rossnagel — Institute of Experimental and Applied Physics, University of Kiel, Germany

Recent research on the layered semiconductor $2H$-MoS_2 has been concentrated on MoS_2 monolayers: In contrast to the bulk crystal, MoS_2 monolayers are direct bandgap semiconductors without an inversion center, making them an appropriate material for valleytronic devices with hot carrier lifetimes in the picosecond regime. However, $2H$-MoS_2 surfaces could be equally exciting: Due to the symmetry breaking at the surface or a decoupling of the topmost sandwich, similarities to monolayers seem possible. For an investigation of this system, time- and angle-resolved photoelectron spectroscopy is the method of choice, as it provides high surface sensitivity and momentum resolution, while enabling us to map electronic processes on their fundamental time scales. Here, we present a $\vec{k}$-resolved study of the transient photoelectron intensity in the conduction band after excitation of $2H$-MoS_2 surfaces with 3.2 eV pump pulses. Momentum-dependent intensity rise times between 30 fs and 150 fs and decay times of several 100 fs allow us to identify direct electronic excitations and to track the electrons' relaxation pathway into the lowest energy states. The conduction band minima are finally depopulated within ∼1 ps. Possible explanations for this observation – such as diffusion processes, optical electron-hole recombination and trapping in defect states – are discussed.

TT 80.7 Wed 16:45 MA 005

Charge carrier trapping and electron-phonon coupling in MoS_2 revealed by μ-Raman spectroscopy — Bastian Miller[1,2], Eric Parzinger[1,2], Alexander Holleitner[1,2], and •Ursula Wurstbauer[1,2] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 München, Germany

Two-dimensional layered van-der Waals materials are of increasing interest for fundamental research as well as device applications in the areas of electronics, spin- and valleytronics, optoelectronics, and sensing. We utilize power and gate voltage dependent non-resonant and resonant μ-Raman spectroscopy on dual-gate field-effect transistor devices to study doping effects, e-ph coupling and the impact of trap states in mono-, bi- and few layer MoS_2. In non-resonant Raman measurements we observe a strong power- and gate voltage dependence of zone-center Raman modes with contrasting behavior for mono- and bilayer MoS_2. Under resonant excitation, a rich scattering spectra with signatures of multistep scattering processes are observable pointing towards contribution from phonon-phonon and electron-phonon interaction. The origin of the different modes, their dependence on the exciting light energy and evolution with number of layers will be discussed. We acknowledge the financial support by the DFG excellence cluster Nanosystems Initiative Munich (NIM).

TT 80.8 Wed 17:00 MA 005

Newly observed first-order resonant Raman modes in few-layer molybdenum disulfide — •Nils Scheuschner, Roland Gillen, Matthias Staiger, and Janina Maultzsch — Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin

We show measurements of two newly observed first-order Raman modes in few-layer MoS_2 with phonon energies of 286 cm^{-1} and 471 cm^{-1}. These modes are strongly resonant and appear only when using excitation energies above ≈ 2.4 eV. At 2.7 eV, their intensity is comparable to the second-order Raman modes; their absence thus provides an easy and accurate method to identify single-layer MoS_2. At UV excitation, the intensity of the new modes is even larger than the typically examined A_1'/A_{1g} and E'/E_g modes. We provide a systematic analysis of the phonon modes, their symmetries, and their frequencies in few-layer materials, including the newly observed modes.

TT 80.9 Wed 17:15 MA 005

Near-field microscopy and nano-FTIR spectroscopy on monolayer MoS2 grown on periodically poled LiNbO3 — •Georg Ulrich[1], Piotr Patoka[1], Peter Hermann[2], Bernd Kästner[2], Ariana Nguyen[3], Tom Scott[4], Arne Hoehl[2], Ludwig Bartels[3], Peter Dowben[4], Gerhard Ulm[2], and Eckart Rühl[1] — [1]Physikalische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, Berlin, 10587 Berlin, Germany — [3]Department of Chemistry, U California Riverside, Riverside, CA 92521, USA —

[4]Department of Physics and Astronomy, U Nebraska, Lincoln, NE 68588-0299 USA

Coupling of synchrotron radiation from the Metrology Light Source to a scanning near-field optical microscope (SNOM) has emerged as a possibility for highly sensitive spectroscopic investigations in the mid-infrared regime [1]. It also allows the simultaneous collection of topographic information and optical response from the samples with a spatial resolution below 30 nm. Here we will present the results of nano-FTIR spectroscopy and near-field imaging of monolayer MoS2 islands on a periodically poled lithium niobate (PPLN) sample using synchrotron radiation in the infrared regime and tunable CO2 laser radiation, respectively. The results show the influence of the ferroelectric polarization of the PPLN structure on the MoS2 semiconductor which enhances the surface polarization of the ferroelectric domains only in one direction. [1] P. Hermann et al., Opt. Express 22, 17948 (2014)

TT 80.10 Wed 17:30 MA 005

Growth and Characterization of Epitaxial Single-Layer MoS_2 on Au(111) — •Jill Miwa, Søren Ulstrup, Signe Sørensen, Maciej Dendzik, Antonija Grubišić Čabo, Marco Bianchi, Jeppe Vang Lauritsen, and Philip Hofmann — Dept. of Physics & Astronomy, Aarhus University, Aarhus, Denmark

We present a method for synthesizing epitaxial single-layer MoS_2 on the (111) face of Au. Using scanning tunnelling microscopy (STM) and low energy electron diffraction, the evolution of the growth is followed from nanoscale single-layer MoS_2 islands to a robust high quality epitaxial MoS_2 layer that is stable in air. We investigate the electronic structure of epitaxial single layer MoS_2 by angle resolved photoemission spectroscopy. Pristine and potassium-doped layers are studied in order to gain access to the conduction band. The potassium-doped layer is found to have a (1.39±0.05) eV direct band gap at $\bar{K}$ with the valence band top at $\bar{\Gamma}$ having a significantly higher binding energy than at $\bar{K}$. A pronounced moiré superstructure of the epitaxial system observed in STM does not lead to the presence of observable replica bands or minigaps. The degeneracy of the upper valence band at $\bar{K}$ is found to be lifted by the spin-orbit interaction, leading to a splitting of (145±4) meV. Finally, it is shown that the potassium doping does not only lead to a rigid shift of the band structure but also to a distortion, giving rise to the possibility of band structure engineering in single-layers of transition metal dichalcogenides.

TT 81: Electronic Structure Theory: Many-Body Effects (organized by O)

Time: Wednesday 18:15–21:00 Location: Poster A

TT 81.1 Wed 18:15 Poster A

Spin Entanglement in Atoms and Molecules — •Stefano Pittalis[1], Filippo Troiani[1], Carlo Andrea Rozzi[1], and Giovanni Vignale[2] — [1]Istituto Nanoscienze, Consiglio Nazionale delle Ricerche, Modena, Italy — [2]Department of Physics, University of Missouri, Columbia, Missouri, USA

We investigate spin entanglement in many-electron systems within the framework of density functional theory. We show that the entanglement length of a Kohn-Sham system, which is extracted from the spatial dependence of the local concurrence, is a sensitive indicator of atomic shells, and reveals the character, covalent or metallic, of chemical bonds. These findings shed light on the remarkable success of modern density functionals, which tacitly employ the entanglement length as a variable. This opens the way to further research on entanglement-based functionals.

TT 81.2 Wed 18:15 Poster A

The role of the quantum well states in the oscillating behavior of the magnetic anisotropy energy and the orbital moment anisotropy — •Leonid Sandratskii — Max Planck Institute of Microstructure Physics, Halle, Germany

We report detailed first-principles theoretical study of the correlated behavior of the magnetic anisotropy energy and the orbital moment anisotropy as a function of the thickness of the ferromagnetic films. The role of the quantum well states in the formation of the oscillations is discussed. The analysis of the contributions of different points in the 2D Brillouin zone is performed. The special role of the surface layer is considered. The symmetry of the quantum mechanical problem is studied. It is shown that the electronic states possess transversal components of the orbital moment that compensate each other after summation over the Brillouin zone.

TT 81.3 Wed 18:15 Poster A

Ab initio calculation of the first order Raman spectrum of graphene and graphite — •Albin Hertrich, Caterina Cocchi, Pasquale Pavone, and Claudia Draxl — Department of Physics, Humboldt-Universität zu Berlin, Germany

Raman scattering produced by fluctuations of the dielectric function caused by phonons is an important non-destructive method for characterizing carbon-based materials. By adopting a fully ab initio approach, we compute the first order Raman spectrum of graphene and graphite using the full-potential all-electron density-functional-theory (DFT) package exciting [1]. This code is based on the augmented plane-waves approach and allows for the calculation of both phonon-dispersion curves, within the frozen-phonon approximation, and frequency-dependent dielectric tensors, from time-dependent DFT and the Bethe-Salpeter equation. Starting from these ingredients, the first-order Raman scattering intensity (G peak) within the adiabatic approximation is obtained from the derivative of the dielectric function with respect to the normal coordinates of the optical phonons at the Γ point of the Brillouin zone and the vibrational matrix element. Our results are interpreted and discussed in comparison with the existing literature.

[1] A. Gulans *et al.* J. Phys.: Condens. Matter **26** (2014) 363202

TT 81.4 Wed 18:15 Poster A

Thermoelectric clathrates: stability of the $Ba_8Al_xSi_{46-x}$ and $Sr_8Al_xSi_{46-x}$ compounds — •Maria Troppenz, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

On the search for high-efficiency thermoelectric materials, promising candidates are clathrate compounds. Their cage-like structure, capable of containing guest atoms, allows for exploiting the idea of the phonon-glass electron-crystal, proposed as a way to reach a large figure of merit.

In this work, we focus on the clathrates $Sr_8Al_xSi_{46-x}$ and $Ba_8Al_xSi_{46-x}$. In contrast to the well-studied Ga-Ge based clathrates, Al-Si clathrates are of technological interest in terms of price, weight, and low environmental impact. The use of Sr and Ba as guests is motivated by the glass-like conductivity of $Sr_8Ga_{16}Ge_{30}$ and the high thermoelectric efficiency of $Ba_8Ga_{16}Ge_{30}$. The electronic transport properties are optimized at the Zintl composition, corresponding to $x = 16$. However, it has not been possible to synthesize samples with $x > 10$ for Sr or $x > 15$ for Ba [1].

We explore the structural stability of the compositional range $0 \leq x \leq 16$ as well as the stability against competing phases that are observed in experiments (e.g. $SrAl_2Si_2$). Due to the large number of substitutional configurations we resort to a cluster expansion based on accurate calculations of a subset of substitutional configurations.

[1] J.H. Roudebush, N. Tsujii, A. Hurtando, H. Hope, Y. Grin, and S.M. Kauzlarich, *Inorg. Chem.* **51**, 4161 (2012).

TT 81.5 Wed 18:15 Poster A

Atomistic Modeling of Optical Coefficients in Layered Materials — •Christian Vorwerk, Caterina Cocchi, and Claudia Draxl — Humboldt Universität zu Berlin and IRIS Adlershof, 10099 Berlin, Germany

The optical properties of a material are fully determined by the complex dielectric tensor. Comparison with measured data however, requires accounting for the experimental setup. This is in particular important for molecular materials, owing to their anisotropic nature.

We apply a 4x4-matrix formalism [1] to calculate optical coefficients of layered anisotropic materials, combining *ab initio* calculations of the dielectric tensor with the solution of Maxwell's equations. This approach [2] allows us to investigate the impact of polarization and incidence angle of the incoming light beam on the spectra of layered materials, having a specific orientation with respect to the substrate. We apply the formalism to optical as well as to X-ray absorption spectra, computing the full dielectric tensor with the all-electron full-potential

code `exciting` [3] by means of many-body perturbation theory. Our prototypical target systems are different polymorphs of sexithiophene, crystals of functionalized pentacenes, self-assembled monolayers of azobenzenes, and more.

[1] P. Yeh, Surf. Sci. 96, 41 (1980). [2] P. Puschnig and C. Ambrosch-Draxl, Adv. Eng. Mater. 8, 1151 (2006). [3] A. Gulans et al., J. Phys.: Condens. Matter 26, 363202 (2014).

TT 81.6 Wed 18:15 Poster A

The Novel Materials Discovery (NoMaD) Repository — •Evgeny Blokhin[1], Fawzi Mohamed[2], Karsten Hannewald[1], Luca Ghiringhelli[2], Pasquale Pavone[1], Christian Carbogno[2], Johann-Christoph Freytag[3], Matthias Scheffler[2], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik und IRIS Adlershof, Zum Großen Windkanal 6, 12489 Berlin — [2]Fritz Haber Institute of the Max Planck Society, Theory Department, Faradayweg 4-6, 14195 Berlin — [3]Humboldt-Universität zu Berlin, Institut für Informatik, Rudower Chaussee 25, 12489 Berlin

Since many years our community is producing an enormous amount of data by CPU-intensive calculations. Most of these data are not used, although the information content is significant. We propose to change our scientific culture following the idea of open access. The NoMaD Repository (https://nomad-repository.eu) was established to host, organize, and share materials data. NoMaD also copes with the increasing demand of storing scientific data and making them available for longer periods. NoMaD facilitates research groups to share and exchange their results. Upload of data is possible without any barrier. Results are accepted in their raw format as produced by the underlying electronic-structure package. At present, the repository is being filled with results for inorganic and organic semiconductors, catalysis and corrosion, optoelectronics, thermoelectrics, and biophysics. These areas will be continuously complemented by others.

TT 81.7 Wed 18:15 Poster A

Acoustic magnons in the long-wavelength limit: resolving the Goldstone violation in many-body perturbation theory — •Mathias C.T.D. Müller, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Ferromagnetic materials exhibit a spontaneously broken global rotation symmetry in spin space leading to the appearance of massless quasiparticles (zero gap) in the long-wavelength limit. These magnons are formed by the correlated motion of electron-hole pairs with opposite spins, which we describe from first principles employing the T-matrix formalism in the ladder approximation within the FLAPW method [1]. Due to approximations used in the numerical scheme, the acoustic magnon dispersion exhibits a small but finite gap at Γ. We analyze this violation of the Goldstone mode and discuss possible correction schemes. One of the correction schemes, which involves an adjustment of the Kohn-Sham (KS) exchange splitting, is motivated by the spin-wave solution of the one-band Hubbard model. The new exchange splittings turn out to be closer to experiment. We present corrected magnon spectra for Co, Ni, and Fe. In addition, we discuss an approach that implements the magnetic susceptibility using a renormalized Green function instead of the KS one. The latter, much more expensive approach is expected to fulfill the Goldstone condition without correction.

[1] E. Şaşıoğlu *et al.*, Phys. Rev. B **81**, 054434 (2010); C. Friedrich *et al.* Top. Curr. Chem. **347**, 259 (2014).

TT 81.8 Wed 18:15 Poster A

Electronic Structure of Hybrid Materials by Means of Self-Consistent *GW* — •Nora Salas-Illanes and Claudia Draxl — Humboldt-Universität zu Berlin, Institut für Physik, Theoretische Festkörperphysik, Zum Großen Windkanal 6, 12489 Berlin

Nano-structured hybrid materials, typically consisting of two or more components that exhibit different nature, are very promising for optoelectronic applications. Unexpected new electronic properties can arise in these systems, which are absent in either of the building blocks. Unfortunately, state-of-the-art electronic-structure methods are not well suited or can even badly fail for such interfaces.

For a large number of materials, DFT provides accurate results for most ground-state properties. However, in order to obtain realistic results of electronic excitations, we have to go beyond DFT, using many-body perturbation theory (MBPT). State-of-the-art MBPT calculations are performed using the quasiparticle approach in the GW approximation.

In principle, the GW approach requires the self-consistent solution of the Hedin equations. However, most of the up-to-date calculations are performed using the results of the first iteration (one-shot GW). Unfortunately, this procedure cannot be used for obtaining accurate results for hybrid materials where, instead, some kind of self-consistent GW needs to be employed.

We implemented the quasi-particle self-consistent GW scheme in the all-electron full-potential code **exciting**. We present here the first results of our implementation for selected prototype materials.

TT 81.9 Wed 18:15 Poster A

Size-dependent optical gaps of Cu chalcogenide nanocrystals from *GW* and the Bethe-Salpeter equation — •Sabine Körbel[1,2], Miguel Alexandre Lopes Marques[1,2,3], and Silvana Botti[4,2,3] — [1]Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Université Claude Bernard Lyon 1, France — [3]European Theoretical Spectroscopy Facility — [4]Friedrich-Schiller-Universität Jena, Germany

In semiconductor nanocrystals, quantum confinement, which opens the optical gap with decreasing nanocrystal size, allows to tune the optical absorption edge. Hence, nanoparticles of different sizes may be used in multilayer thin-film solar cells, with each layer consisting of nanocrystals of a different size, absorbing light at a different frequency, therefore enhancing the overall efficiency of the solar cell, all the while using one and the same photovoltaic absorber material. Here we present size-dependent optical gaps of nanocrystals of $Cu_2ZnSn(S,Se)_4$ [CZTS(e)], an earth-abundant semiconductor with a direct optical gap suitable for solar-cell absorbers, calculated with GW and the Bethe-Salpeter equation, and compared to experimental data, where available.

TT 81.10 Wed 18:15 Poster A

2D Metal Dichalocogenides and Oxides for Hydrogen Evolution: A Computational Approach — •Mohnish Pandey[1], Aleksandra Vojvodic[2], Kristian S. Thygesen[1], and Karsten W. Jacobsen[1] — [1]Center for Atomic-scale Materials Design, Department of Physics, Technical University of Denmark, DK - 2800 Kongens Lyngby, Denmark — [2]SUNCAT Center for Interface Science and Catalysis, Department of Chemical Engineering, Stanford University, Stanford, California 94305, United States

We explore the possibilities of hydrogen evolution by basal planes of 2D metal dichalcogenides and oxides in the 2H and 1T phases using the hydrogen binding energy as a computational descriptor. The binding energies are calculated using density functional theory with the BEEF-vdW functional which includes uncertainty estimates on the calculated binding energies. For some groups of systems like the Ti, Zr, and Hf dichalcogenides the hydrogen bonding the bonding to the 2H structure is stronger than to the 1T structure while for the Cr, Mo, and W dichalcogenides the behavior is opposite. This is rationalized investigating shifts in the chalcogenide p-levels comparing the two structures.

TT 82: Electronic Structure Theory: General, Method Development (organized by O)

Time: Wednesday 18:15–21:00 Location: Poster A

TT 82.1 Wed 18:15 Poster A

Electron-phonon coupling in the KKR formalism — •Carsten Eberhard Mahr, Christian Franz, Marcel Giar, and Christian Heiliger — Justus-Liebig University, Giessen, Germany

Electron-phonon coupling is one of the main incoherent inelastic scattering mechanisms in a wide variety of crystalline material systems at room temperature. Therefore, it is necessary to incorporate those effects in any realistic calculation of thermoelectric properties. We do so by extending our density functional theory (DFT) based Korringa-Kohn-Rostocker (KKR) Green's function formalism code.

By adding a Fröhlich-type interaction to the Kohn-Sham Hamiltonian which corresponds to the previously calculated Green's function G_{ee} containing the electron-electron interaction in e.g. local density approximation (LDA), we can compute the dressed propagator through Dyson's equation as $G = G_{\mathrm{ee}} + G_{\mathrm{ee}} \cdot \Sigma_{\mathrm{eph}} \cdot G$. The self-energy Σ_{eph} is treated in Self-Consistent First Born Approximation (SCFBA), which may be obtained using a perturbative diagrammatic approach within Keldysh NEGF formalism.

We give transformed representations of the beforementioned relations and quantities for bulk calculations in the KKR 'basis' set. Based thereupon, central formulas for non-equilibrium transport in our calculational scheme are presented.

TT 82.2 Wed 18:15 Poster A

SEMT: An Orthogonal and Localized Basis-Set for All-electron Density Functional Theory — •Andrea Nobile and Stefan Blügel — Peter Grünberg Institute (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH and JARA, Jülich, Germany

Employing all-electron methods for simulations by density functional theory (DFT) allows for unbiased, highly accurate solutions of the Kohn-Sham equations. Current popular all-electron schemes like FLAPW+LO and APW+LO use a basis set that is not localized in real space and as a consequence the resulting Hamiltonian is dense. These basis sets are non-orthogonal thereby posing constraints on the choice of the eigensolver and on the usage and development of alternative, less than cubic scaling convergence schemes.

We tackle the localization and orthogonality problem by combining spectral elements with muffin-tin spheres. The introduced method, that we call spectral-element-muffin-tin (SEMT), produces a basis set that is localized and numerically orthogonal by construction.

When compared to pure spectral element methods, our basis needs a substantially smaller number of degrees of freedom per atom. The strength of the SEMT method is in the combination of all-electron, real space, sparsity and orthogonality. We demonstrate the method with our implementation (Velvet) on some elemental materials by comparing the results with FLAPW+LO calculations.

TT 82.3 Wed 18:15 Poster A

Electron-phonon relaxation times from first principle calculations — •Florian Rittweger[1,2], Nicki F. Hinsche[1], and Ingrid Mertig[1,2] — [1]Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, DE-06120 Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, DE-06120 Halle

Electron-phonon interaction (EPI) is usually related to the phenomenon of superconductivity. Besides these studies the influence of the EPI on transport properties became popular in the last years.

While ARPES measurements offer experimental access to the EPI, theoretical approaches are based on the calculation of the electron-phonon matrix elements. The latter leads either to the calculation of the complex electron-phonon self-energy and therefore the renormalization of the electronic band structure or to the estimation of the electron-phonon coupling strength λ and the state-dependent relaxation time $\tau_{\mathbf{k}}$. The k-dependence of τ enters the Boltzmann equation for the computation of transport properties like the electrical conductivity, thermal conductivity and the thermopower beyond the relaxation time approximation typically used.

We calculate the EPI using linear response density functional perturbation theory and present first results and discussions for simple metals.

TT 82.4 Wed 18:15 Poster A

How Molecules Interact Through Nanostructures — •Mausumi Chattopadhyaya and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Berlin, Germany

Molecules often interact and assemble in the presence of environments, such as solvents, surfaces, or nanostructures. While in the gas phase intermolecular interactions are fairly well understood, much less is known about intermolecular interactions in polarizable environments. To shed some light into this matter, we have investigated the interaction between aromatic molecules through a range of nanostructures, including graphene, h-BN, fullerenes, carbon nanotubes, and phosphorene. In each of these cases, we have computed the non-additive interaction terms by using density-functional theory with many-body dispersion interactions (DFT+MBD method [1,2]). We found that in most of the cases the intermolecular interaction energy decreases due to the presence of a nanostructure, as expected from classical electrodynamics. However, for sufficiently polarizable nanostructures, we observe a regime in which the interaction energy increases due to non-trivial quantum-mechanical fluctuations of electric dipoles. [1] Phys. Rev. Lett. 108, 236402 (2012); [2] J. Chem. Phys. 140, 18A508 (2014).

TT 82.5 Wed 18:15 Poster A

Precise dynamical response functions in all-electron methods: application to the RPA correlation energy — Markus Betzinger, •Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany

The main obstacle in calculating dynamical response functions in practice is their slow convergence with respect to the basis-set size and the number of unoccupied bands. We showed in Refs. [1,2] for the static Kohn-Sham (KS) density response in the all-electron FLAPW method that an incomplete-basis-set correction (IBC) gives rise to a much better convergence behavior. The IBC contains a basis response term that provides response contributions that lie outside the Hilbert space spanned by the original basis. These contributions, therefore, incorporate to some extent an infinite number of states. We present an extension of the IBC to the frequency domain and demonstrate that precise RPA response functions can be obtained already with small basis-set sizes and few numbers of unoccupied states. As an example, we apply the correction to the RPA correlation energy of KS density-functional theory, whose central ingredient is the RPA response function.

[1] M. Betzinger *et al.*, Phys. Rev. B **85**, 245124 (2012).
[2] M. Betzinger *et al.*, Phys. Rev. B **88**, 075130 (2013).

TT 82.6 Wed 18:15 Poster A

RPA spectra from a combination of tetrahedron method and Wannier interpolation — •Johannes Kirchmair, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The polarization function within the random-phase approximation (RPA) describes the response of the electron density due to perturbations of the effective potential and is one of the key quantities in many-body perturbation theory. For example, it is employed in the calculations of *GW* quasiparticle energies, the RPA correlation energy, the Hubbard *U* parameter, but also in phonon calculations. Very often, practical calculations of the polarization function suffer from severe convergence problems. The convergence with respect to unoccupied states has recently been discussed a lot in literature and correction schemes have been proposed. Another problem is the summation over, in principle, infinitely many k points. The standard method, the so-called tetrahedron method, uses a geometrical interpolation in the three dimensions of reciprocal space that can be understood as the analog of linear interpolation in one dimension. This fast and reliable method, however, shows slow convergence of the spectral properties especially for small frequencies. In this work, we propose to take these low-energy virtual excitations from a Wannier-interpolated band structure. The Wannier interpolation is seamlessly combined with the tetrahedron method, which then takes care of the high-energy virtual excitations. We show test calculations and first results for RPA spectra.

TT 82.7 Wed 18:15 Poster A

Calculation of electron energy loss spectra for resistive switching oxides from first principles — •Roman Kováčik[1,2] and Marjana Ležaić[2] — [1]I. Physikalisches Institut, RWTH Aachen and JARA, 52056 Aachen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Calculation of the energy-loss near-edge structure (ELNES) of electron energy loss spectra (EELS) is implemented within the density functional theory framework using the full potential linearized augmented planewave (FLAPW) approach in the FLEUR code (`www.flapw.de`). The double differential cross-section is evaluated using the full relativistic treatment of incoming electrons and the transition matrix elements allowing arbitrary transitions (beyond the dipole approximation) following the formalism of Jorissen (PhD thesis, 2007). We present ELNES calculations of EELS on complex oxides with a promising application in resistive switching, such as Sr-rich phases in $SrTiO_3$. Support from the DFG (SFB917-Nanoswitches) is gratefully acknowledged.

TT 83: Graphene: Adsorption, Intercalation and Doping (organized by O)

Time: Wednesday 18:15–21:00 Location: Poster A

TT 83.1 Wed 18:15 Poster A

Defects and oxygen adatoms on graphene — •Jan Gesenhues and Michael Rohlfing — Institut für Festkörpertheorie, Universität Münster, 48149 Münster, Germany

Oxygen adatoms on graphene are one of the ingredients of graphene oxide and are being discussed as building blocks to open a band gap in the Dirac cone of graphene. In our work we study graphene and oxygen adatoms within the theoretical framework of Tight-Binding and Density Functional Theory (DFT). The SIESTA program was used to carry out the DFT calculations.

In order to study defects in the graphene-layer a supercell approach is used. We take a closer look at the 5-7 defect and its effect on the electronic structure, in particular on the local density of states near the Fermi level. Furthermore we investigate the absorbtion of a single oxygen atom on the graphene-layer. Structure optimisations for various unit-cell sizes show that the oxygen atom equilibrium position is approximatly 2 Å above the layer, also resulting in a perpendicular displacement of the surrounding carbon atoms of a few 0.1 Å. The effetcs on the electronic structure are studied in comparison with the undisturbed system via the (local) density of states.

TT 83.2 Wed 18:15 Poster A

High Energy Ion Irradiation of Graphene — Philipp Ernst[1], •Tobias Foller[1], Oliver Ochedowski[1], Roland Kozubek[1], Johannes Hopster[1], Jan Weber[2], Thorsten Balgar[2], and Marika Schleberger[1] — [1]Fakultät für Physik and CeNIDE, Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Fakultät für Chemie and CeNIDE, Universität Duisburg-Essen, 45117 Duisburg, Germany

In this presentation we show that single high energetic ions can be used as a tool to locally modify the properties of graphene. For this graphene samples are irradiated with swift heavy ions (typical kinetic energies in the rage of 100 MeV) and slow highly charged ions (potential energies up to 45 keV). By combining various analytical techniques like AFM, TEM, and Raman spectroscopy it is shown that depending on the irradiation parameters (ion energy, angle of incidence, choice of substrate for graphene) various modifications like local defective areas, pores in form of origami-like foldings and even doping can be introduced into the graphene sheet. Remarkably graphene field-effect measurements revealed that irradiation with swift heavy ions under perpendicular incidence with small fluences doubles the mobility of holes compared to the unirradiated sample. In contrast to this, irradiation with highly charged ions decrease the mobility. In this case defects are created which are subsequently hydrogenated as strongly suggested by sum frequency generation spectroscopy.

TT 83.3 Wed 18:15 Poster A

Initial stages of hydrogen intercalation of epitaxial graphene studied by XPS and LEEM — •Julia Krone, Florian Speck, Felix Fromm, Martina Wanke, and Thomas Seyller — TU Chemnitz, Institut für Physik, Reichenhainer Straße 70, 09126 Chemnitz, Germany

During graphitization of SiC(0001) surfaces, a buffer layer (BL) is formed at the interface between graphene and the substrate. The BL is a graphene-like layer covalently bound to the SiC [1]. Hydrogen intercalation underneath the BL has been shown to decouple it from the substrate, thus converting it into quasi-freestanding monolayer graphene (QFMLG) [2]. This modification of the interface results in improved charge carrier mobility as compared to regular epitaxial graphene on SiC [3], making it an interesting material for electronic applications. Investigation of short-time annealing of the BL in molecular hydrogen could help to elucidate the initial stages of hydrogen intercalation and BL decoupling. In this work, we employ a combination of X-ray photoelectron spectroscopy, low-energy electron microscopy and low-energy electron diffraction to study the onset of QFMLG formation.

[1] K. V. Emtsev *et al.*, Phys. Rev. B **77**, 155303 (2008).
[2] C. Riedl *et al.*, Phys. Rev. Lett. **103**, 246804 (2009).
[3] F. Speck *et al.*, Appl. Phys. Lett. **99**, 122106 (2011).

TT 83.4 Wed 18:15 Poster A

XPS-investigation of the interaction of Lanthanides with epitaxial graphene — •Sarah Roscher, Martina Wanke, and Thomas Seyller — Institut für Physik, TU Chemnitz, Reichenhainer Sraße 70, D-09126 Chemnitz, Germany

Large-scale epitaxial graphene on silicon carbide is promising for electronic applications. Recently, interface engineering by intercalation of various elements underneath the buffer layer has been studied by several groups and it was demonstrated that elements of the Lanthanides are able to intercalate through epitaxial graphene [1-3]. In this study, erbium was deposited onto different graphene layers epitaxially grown on SiC(0001) and subsequently annealed in a temperature range of 300-950°C. X-ray photoelectron spectroscopy (XPS) was employed to determine the chemical composition of the sample, the intercalation, and the amount of doping. The XPS data indicate that subsequent heating to 850°C results in partial intercalation of the buffer layer. Because of erbium's high reactivity the influence of oxygen on the sample preparation demanded particular attention.

[1] S. Schumacher et al., Nano Lett. 13 (2013) 5013.
[2] S. Watcharinyanon et al., Graphene 2 (2013) 66.
[3] L. Huang et al., Appl. Phys. Lett. 99 (2011) 163107.

TT 83.5 Wed 18:15 Poster A

Structure and thermodynamic stability of graphene oxide — •Sebastian Gsänger and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

A large set of possible atomic configurations of graphene oxide with different composition and coverage were investigated by density functional theory. The adsorption of hydroxyl groups and the formation of epoxides and endoperoxides was systematically evaluated. In a first series of calculations the mutual interaction and the preferred relative position of pairs of adsorbates was determined. Based on these results, promising low-energy adsorption pattern at high coverage were derived and their thermodynamic stability was analyzed in terms of a surface phase diagram. Finally, the possibility for formation of 1,4-endoperoxides on graphene oxide was investigated in detail.

TT 83.6 Wed 18:15 Poster A

Investigation of the molecular doping of graphene on 6H-SiC(0001) — •Christian Raidel[1], Christian Heidrich[1], Julia Krone[1], Florian Speck[1], Peter Wehrfritz[1], Felix Fromm[1], Roland J. Koch[1], Peter Robaschik[2], Francisc Haidu[2], Ovidiu Gordan[2], Zoran Mazej[3], Dietrich R. T. Zahn[2], Thomas Seyller[1], and Martina Wanke[1] — [1]Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany — [2]Halbleiterphysik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany — [3]Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

Graphene is characterized by two linear bands crossing each other at the K-point of the hexagonal Brillouin zone. In neutral graphene, the

Fermi level lies exactly at the crossing point where the density of states is zero. For certain applications, it is desirable to choose both charge carrier type and density which can be accomplished by electrostatic gating or doping. While substitutional doping alters the graphene lattice, charge transfer doping using adsorbates keeps the lattice intact.

In this work, we investigate charge transfer doping of graphene on 6H-SiC(0001) by organic molecules. Angle-resolved photoelectron spectroscopy (ARPES) was used to determine the position of the Dirac point and thus charge carrier type and density. It was observed that fluorinated fullerenes, mainly C60F48 can effectively induce p-type doping [1]. Thereby, the charge transfer is influenced by electron affinity of the adsorbed molecule and by the work function of the graphene, which was investigated in these studies. A model for the doping efficiency [1] of the various adsorbates was tested.

[1] Tadich, et al., APL 102, 241601 (2013)

TT 83.7 Wed 18:15 Poster A

Theoretical NMR signatures of water and ice on graphene — •Achraf Jaadouni, Eva Rauls, Wolf Gero Schmidt, and Uwe Gerstmann — University of Paderborn, Paderborn Germany

Since the discovery of graphene the adsorption of water has been discussed as a possibility for doping [1], while changing the electron mobility surprisingly little. Theoretical studies have shown that the electronic properties of the resulting system strongly depends on the microscopic details of the substrate [2].

In this theoretical work we investigate the influence of thin layers of ice using density functional theory (DFT) whereby van-der-Waals interaction has been taken into account. We demonstrate that an adsorption of at least two layers of ice on free standing graphene results in a charge transfer between the ice and graphene layers and, thus, can lead to a doping of graphene. The sign of the charge transfer and by this the type of doping, however, depends on the orientation of the water molecules. As a consequence, a mixture of two phases can result in a cancellation of the doping effect. Whereas the two configuration differ only slightly in total energies, the NMR chemical shifts calculated for both types of nuclei, O as well as H, are significantly different. Hence, a control of the orientation of the ice layers should be experimentally possible via nuclear magnetic resonance (NMR).

[1] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva, A.A. Firsov, Science 306, 666 (2004).

[2] T.O. Wehling, A.I. Lichtenstein, and M.I. Katsnelson, Appl. Phys. Lett. 93, 202110 (2008).

TT 84: Focus Session: Nanoscopic Superconducting Heterostructures

In recent years superconducting nanostructures were the subject of intensive experimental and theoretical research activities. Boosted by the experimental observation of triplet superconductivity in heterostructures of non-collinear ferromagnets and superconductors, numerous novel applications have been suggested. Triplet supercurrents are simultaneous, dissipationless charge and spin currents. The magnetically induced spin-dependent density of states in superconducting films can carry spin currents over ultra long distances or yield giant thermoelectric effects, which might be useful in spintronic or caloritronic applications. Furthermore nanostructured high-temperature superconductors might open new possibilities to taylor unconventional transport properties. This Focus Session will highlight the most recent progress in this internationally active field.

Organizers: Wolfgang Belzig and Elke Scheer (Uni Konstanz)

Time: Thursday 9:30–13:15 Location: H 0104

Invited Talk TT 84.1 Thu 9:30 H 0104

Creating and Manipulating Nonequilibrium Spins in Nanoscale Superconductors — Michael J. Wolf[1], Florian Hübler[1,2], Stefan Kolenda[1], Christoph Sürgers[3], Gerda Fischer[3], Hilbert von Löhneysen[2,3], and •Detlef Beckmann[1] — [1]Institut für Nanotechnologie, Karlsruher Institut für Technologie — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie — [3]Physikalisches Institut, Karlsruher Institut für Technologie

We report on nonlocal transport in superconductor hybrid structures, with ferromagnetic as well as normal-metal tunnel junctions attached to the superconductor. In the presence of a strong Zeeman splitting of the density of states, we find signatures of spin transport over distances of several μm [1], exceeding other length scales such as the coherence length, the normal-state spin-diffusion length, and the charge-imbalance length [2]. Using a combination of ferromagnetic and normal-metal contacts, we demonstrate spin injection from a normal metal, and show a complete separation of charge and spin imbalance [3]. An exchange splitting induced by the ferromagnetic insulator europium sulfide enables spin transport at very small applied magnetic fields, and therefore paves the way to manipulating spin currents by local exchange fields [4].

[1] F. Hübler et al., Phys. Rev. Lett. **109**, 207001 (2012)
[2] F. Hübler et al., Phys. Rev. B **81**, 184524 (2010)
[3] M. J. Wolf et al., Phys. Rev. B **87**, 024517 (2013)
[4] M. J. Wolf et al., Phys. Rev. B **90**, 144509 (2014)

Topical Talk TT 84.2 Thu 10:00 H 0104

Non-Equilibrium Effects in a Josephson Junction Coupled to a Precessing Spin — •Mikael Fogelström — Department of Microtechnology and Nanoscience, Chalmers University of Technology, 42196 Göteborg, Sweden

I will discuss a theoretical study of s-wave superconductors coupled to a classical spin. When an external magnetic field is applied, the classical spin can be driven to precess with the Larmor frequency. This results in a time-dependent boundary condition for the superconducting quasiparticles, with different tunnelling amplitudes for spin-up and spin-down quasiparticles and where the precession produces spin-flip scattering processes. Andreev states develop at the interface with a non-equilibrium population which depend on how the spin is driven. The Andreev states carry a steady-state Josephson current whose current-phase relation could be used for characterising the spin. In addition to the charge transport, a spin current is also generated. This spin current will induce a torque and couple back to the dynamics of the classical spin.

Topical Talk TT 84.3 Thu 10:30 H 0104

Signature of Magnetic-Dependent Gapless Odd Frequency States at Superconductor / Ferromagnet Interfaces — •Jason Robinson — Department of Materials Science, 27 Charles Babbage Road, Cambridge, CB30FS UK

The theory of superconductivity developed by Bardeen, Cooper, and Schrieffer (BCS) explains the stabilisation of electron pairs into a spin-singlet, even frequency, state by the formation of an energy gap below which the density of states (DoS) is zero. At a superconductor interface with an inhomogeneous ferromagnet, a gapless odd frequency superconducting state is predicted in which the Cooper pairs are in a spin-triplet state. Although indirect evidence for such a state has been obtained, the gap structure and pairing symmetry have not so far been determined. In this talk I will present scanning tunnelling spectroscopy of Nb superconducting films proximity coupled to epitaxial Ho. These measurements reveal pronounced changes to the Nb sub-gap superconducting DoS on driving the Ho through a metamagnetic transition from a helical antiferromagnetic to a homogeneous ferromagnetic state for which a BCS-like gap is recovered. The results verify odd frequency spin-triplet superconductivity at superconductor / inhomogeneous magnet interfaces.

15 min. break.

Invited Talk TT 84.4 Thu 11:15 H 0104

Thermoelectric Effects and Spin Injection into Superconductors with Exchange Field — •Tero Heikkilä[1], Mihail Silaev[2,3], Pauli Virtanen[2], Francesco Giazotto[4], Asier Ozaeta[5], and Sebastian Bergeret[5] — [1]Dept Phys, Univ Jyväskylä, Finland — [2]O.V. Lounasmaa Lab, Aalto Univ, Finland — [3]Dept Theor Physics, KTH, Stockholm, Sweden — [4]NEST CNR-INFM and SNS Pisa, Italy — [5]CFM-CSIC and DIPC, San Sebastian, Spain

When a thin superconducting film is exposed to a longitudinal magnetic field or is in proximity to a ferromagnet, an exchange field separating the spin bands emerges in it. For low enough exchange fields superconductivity survives, but its response to external driving is strongly modified. In my talk I will show how at linear response such systems exhibit very strong thermoelectric response with an almost ideal efficiency. For strong driving, this effect creates a spin accumulation that can only relax via thermalization, and therefore at low temperatures has a very long range. Therefore our work explains recent observations of the long-range spin accumulation in spin-split superconductors. When injecting spin from injectors with non-collinear magnetization compared to the exchange field, the spins start to rotate around the latter. I will describe how superconductivity modifies this spin Hanle effect so that the resulting nonlocal magnetoresistance depends on the details of spin relaxation, therefore allowing for probing them.

Topical Talk TT 84.5 Thu 11:45 H 0104

Spin Injection and Relaxation in a Mesoscopic Superconductor — •Marco Aprili[1], Charis Quay[1], Denis Chevalier[1], Clement Dutreix[1], Cristina Bena[2], and Christoph Strunk[3] — [1]Laboratoire de Physique des Solides, CNRS UMR-8502, Bât. 510, Université Paris-Sud, 91405 Orsay Cedex, France — [2]Institut de Physique Théorique, CEA/Saclay, Orme des Merisiers, 91190 Gif-sur-Yvette Cedex, France — [3]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Injecting spin-polarized electrons or holes into a superconductor and removing Cooper pairs creates both spin and charge imbalances. We have investigated the relaxation of the out-of-equilibrium magnetization induced by spin injection. First, we measured the spin and charge relaxation times (t_S and t_Q) by creating a dynamic equilibrium between continuous injection and relaxation, this leads to constant-in-time spin and charge accumulation proportional to their respective relaxation times. Using a mesoscopic "absolute" spin-valve, we obtained t_S and t_Q by probing the difference on the chemical potential between quasiparticles and Cooper pairs. We observed that spin (charge) accumulation dominates at low (high) injection current. This artificially generates spin-charge separation as theoretically first predicted by Kivelson and Rokhsar. Second, we directly measured the spin relaxation time in the frequency space and found $t_S = 1 - 10$ ns consistent with results from constant current injection. Finally, we measured the spin coherence time of the out-of-equilibrium quasi-particles by performing an electron spin resonance experiment.

TT 84.6 Thu 12:15 H 0104

Probing odd-triplet contributions to the long-ranged proximity effect by scanning tunneling spectroscopy — •Simon Diesch[1], Christoph Sürgers[2], Detlef Beckmann[2], Peter Machon[1], Wolfgang Belzig[1], and Elke Scheer[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany

In conventional superconductors, electrons are bound in singlet Cooper pairs, i.e. with opposite spin. More recently, experiments on superconductor-ferromagnet-systems have shown Cooper pairs tunneling through ferromagnetic layers, indicating Cooper pairs of equal spin, thus corresponding to a long-range triplet proximity effect. Most experimental evidence for triplet superconductivity comes from observations of the thickness dependence of the Josephson current through a ferromagnetic barrier, but there is an increasing interest in obtaining direct spectroscopic evidence.

This project aims at analyzing the electronic density of states of a thin diffusive normal metal layer (Ag) coupled to a superconductor (Al) across a ferromagnetic insulator (EuS) using a scanning tunneling microscope in spectroscopy mode at 280 mK. For this purpose, we fabricated EuS films of different thicknesses and acquired spectroscopic data at different magnetic fields. We observe significant broadening of the superconductive energy gap and a variety of sub-gap structures including zero-bias conductance peaks induced by the presence of the ferromagnet.

TT 84.7 Thu 12:30 H 0104

Electronic heat, charge and spin transport in superconductor-ferromagnetic insulator structures — •Sebastian Bergeret — Materials Physics Center (CFM_CSIC), San Sebastian, Spain — Donostia International Physics Center (DIPC), San Sebastian, Spain

It is known for some time that a superconducting (S) film in contact with a ferromagnetic insulator (FI) exhibits a spin-splitting in the density of states (DoS). Recently we have explored different S-FI hybrid structures and predicted novel effects exploiting such spin-splitting of the DoS. In this talk I will briefly discuss (i) a heat valve based on a FI-S-I-S-FI Josephson junction; (ii) a thermoelectric transistor and (iii) the occurrence of a giant thermophase in a thermally-biased Josephson junction.

TT 84.8 Thu 12:45 H 0104

Correlation of 0-π transition with density of states measurements — •Ondrej Vavra[1,2], Petra Högl[3], Jaroslav Fabian[3], Hermann Kohlstedt[2], and Christoph Strunk[1] — [1]Inst. for Experimental and Applied Physics, University of Regensburg, Germany — [2]Nanoelektronik, Technical Faculty, University of Kiel, Germany — [3]Inst. for Theoretical Physics, University of Regensburg, Germany

We report on the proximity induced superconductivity in hybrid SFIFS (Nb-Fe-Al_2O_3-Fe-Nb) and SIFS (Nb-Al_2O_3-Fe-Nb) Josephson junctions. Differential conductance curves $dI/dV(V)$ were recorded with the lock-in technique on the SFIFS samples exposed to a small magnetic field that suppresses the critical current I_C. The $dI/dV(V)$ curves reveal a peak at a voltage 2.26 mV which is attributed to the sum of the gaps of individual Nb electrodes ($2\Delta_{Nb}$). Upon increasing iron thickness d_{Fe} a second peak develops at a voltage 1.3 mV which we attribute to the induced superconductivity in the Fe-layers. The peak height difference $|G_{Nb} - G_{Fe}|(d_{Fe})$ oscillates with zero crossings at 2.3 and 2.9 nm, respectively. Qualitatively, the Fe thickness dependence of $dI/dV(V)$ behavior is the same for both SFIFS and SIFS junctions, respectively. The shape of the $|G_{Nb} - G_{Fe}|(d_{Fe})$ curve with its oscillations is similar to the $I_C(d_{Fe})$ curves for Josephson junctions with F-interlayer and to the $T_C(d_{Fe})$ dependencies for the S-F multilayers. These oscillations are observed due to the phase transition from 0 to π and vice-versa. We will discuss the results of deconvolution of $dI/dV(V)$ curves and correlate these data with Fe thickness development of the critical current.

TT 84.9 Thu 13:00 H 0104

Controllable transfer of magnetism in superconducting spin-valve structures — •Matthias Eschrig — Royal Holloway, University of London, UK

During the past 15 years a new field has emerged, which combines superconductivity and spintronics, with the goal to pave a way for new types of devices for applications combining the virtues of both, namely quantum coherence and interference on one side, and spin-selectivity and spin magnetism on the other. The building block of this new "superspintronics" are spin-triplet Cooper pairs, which are generated at the interface between a conventional superconducting and a ferromagnetic material. Non-collinear magnetic inhomogeneity mixes triplet pairs among each other, thus creating long-ranged equal-spin Cooper pairs in the ferromagnet, and non-coplanar inhomogeneity introduces geometric phases giving rise to unusual current phase relations. We discuss recent experiments [1] on superconducting spin-valve structures reporting a controllable transfer of magnetism via equal-spin Cooper pairs. We present theoretical models for for such an effect and discuss its implications for applications.

This work is supported by the Engineering and Physical Science Research Council (EPSRC Grant No. EP/J010618/1).

[1] M.G. Flokstra, N. Satchell, J. Kim, G. Burnell, S.J. Bending, P.J. Curran, S. Langridge, C.J. Kinane, J.F.K. Cooper, M. Eschrig, A. Isidori, N. Pugach, H. Luetkens, T. Prokscha, S. L. Lee, unpublished.

TT 85: Superconductivity: Higgs Modes in Condensed Matter and Quantum Gases (jointly with DY, MA, O)

Time: Thursday 9:30–11:15 Location: H 2053

Invited Talk TT 85.1 Thu 9:30 H 2053

A Brisk Walk through Phase Transitions in Time: Oscillating Order and the Dynamics of Topological Defects — •Dragan Mihailovic — Jozef Stefan Institute, Ljubljana, Slovenia

New techniques in time-resolved optical spectroscopy allow us to investigate phase transitions under controlled, yet highly non-ergodic conditions. The measurement of the temporal evolution of not only single particle and collective excitations, but also topological excitations through the transition lead to a new insight into the emergence of functional properties under non-equilibrium conditions. Experiments on well-known rare earth and transition metal chalcogenides which I will discuss reveal some unexpected phenomena. For example, femtosecond coherent oscillations of the order parameter and the subsequent coherent creation and annihilation of topological defects leads to a transient domain structure which decays through the emission of dispersive Higgs-like amplitude waves [1,2]. Remarkably, if the conditions are right (defined by the material), the topological defects may form an ordered metastable state, which is topologically protected, opening a route to the creation of hidden states [3]. Such switching between states with different charge order occurs at unprecedented speeds and is of potential interest for ultrafast non-volatile memory technology, with either optical or electrical control.

[1] R. Yusupov et al., Nature Phys. **6**, 681 (2010)
[2] D. Mihailovic et al., J. Phys.: Condens. Matter **25**, 404206 (2013)
[3] L. Stojchevska et al., Science **344**, 177 (2014)

TT 85.2 Thu 10:00 H 2053

Nonadiabatic dynamics and coherent control of nonequilibrium superconductors — •Andreas Schnyder[1], Holger Krull[2], Dirk Manske[1], and Götz Uhrig[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Lehrstuhl für Theoretische Physik I, Technische Univerität Dortmund, Otto-Hahn Straße 4, 44221 Dortmund, Germany

Inspired by recent THz pump-THz probe experiments on NbN films [1], we theoretically study the pump-probe response of nonequilibrium superconductors coupled to optical phonons. For ultrashort pump pulses a nonadiabatic regime emerges, which is characterized by amplitude oscillations of the superconducting gap [2] and by the generation of coherent phonons [3]. Using density-matrix theory as well as analytical methods, we compute the pump-probe response of the superconductor in the nonadiabatic regime and determine the signatures of the order parameter and of the phonon oscillations in the pump-probe conductivity. We find that the nonadiabatic dynamics of the superconductor reflects itself in oscillations of the pump-probe response as a function of delay time between pump and probe pulses [4]. We also consider two-band superconductors and study the interplay of the two amplitude oscillations of the two gaps.

[1] R. Matsunaga et al., PRL 111, 057002 (2013)
[2] E. A. Yuzbashyan et al., PRL 96, 097005 (2006)
[3] A. P. Schnyder, D. Manske, and A. Avella, PRB 84, 214513 (2011)
[4] H. Krull, D. Manske, G. S. Uhrig, and A. P. Schnyder, PRB 90, 014515 (2014)

TT 85.3 Thu 10:15 H 2053

THz Investigations of the Higgs Amplitude Mode in Superconducting Thin Films — •Martin Dressel[1], Uwe S. Pracht[1], Daniel Sherman[2], Aviad Frydman[2], Boris Gorshunov[1,3,4], Pratap Raychaudhuri[5], Nandini Trivedi[6], and Assa Auerbach[7] — [1]1. Phys. Inst., Universtät Stuttgart — [2]Phys. Dept., Bar Ilan University, Ramat Gan, Israel — [3]General Physics Inst, RUS, Moscow, Russia — [4]Moscow Inst. Phys. and Techn., Dolgoprudny, Russia — [5]Tata Inst. Fund. Res., Mumbai, India — [6]Phys. Dept., Ohio State University, Columbus, U.S.A. — [7]Phys. Dept., Technion, Haifa, Israel

We have measured thin superconducting films of various degrees of disorder by THz spectroscopy in order to investigate the optical conductivity at low temperatures. While the properties of weakly disordered superconductors, such as NbN or InO, can be well described by the BCS theory, significant deviations are observed as disorder increases towards the superconductor-insulator transition. On both sides of the transition, tunneling spectroscopy determines a finite pairing gap 2Δ. In contrast, the threshold frequency for the dynamical conductivity, which in BCS theory is associated with the gap, vanishes critically toward the superconductor insulator transition. Here we can identify an excess optical spectral weight below 2Δ as the first unambiguous evidence of a well-defined Higgs amplitude mode observed in a superconductor.

TT 85.4 Thu 10:30 H 2053

Magnon-Interactions and Higgs Mode in 2D Quantum Antiferromagnets from Raman Scattering — •Simon Weidinger and Wilhelm Zwerger — Physik-Department, Technische Universität München, 85747 Garching, Deutschland

We present a theory for Raman scattering on 2D quantum antiferromagnets. The microscopic Fleury-Loudon Hamiltonian is expressed in terms of an effective O(3)- model. Well within the Neel ordered phase, the Raman spectrum contains both a two-magnon and two-Higgs contribution which are calculated diagrammatically. The spectrum is dominated by a broad two-magnon peak but it is hardly affected by the Higgs-mode of the 2D Neel ordered state. This is a consequence of the momentum dependence of the Raman vertex in the relevant B_{1g} symmetry. The resulting nontrivial spectrum, which has the antiferromagnetic exchange coupling as a single parameter, is in very good agreement with experiments on undoped cuprates.

TT 85.5 Thu 10:45 H 2053

Higgs Mechanism in Three-Dimensional Topological Superconductors and Anomalous Hall Effect in Zero Magnetic Field — •Flavio Nogueira and Ilya Eremin — Theoretische Physik III, Ruhr-Universität Bochum

We discuss the peculiar nature of Higgs mechanism in an effective field theory for three-dimensional topological superconductors. The effective theory features two order parameters associated to the two chiral fermion species in the system. The resulting electrodynamics of such a topological superconductor exhibits a topological magnetoelectric effect with an axion field given by the phase difference of the order parameters. As consequence, the London regime is highly non-linear and anomalous Hall effect in the absence of an external magnetic field occurs. In this anomalous Hall effect the generated current transverse to an applied electric field changes sign with the temperature. We also discuss the scaling behavior of the penetration depth near the transition temperature, which is also shown to exhibit a scaling exponent that is crucially influenced by the axion term, varying continuously as function of the average phase difference.

TT 85.6 Thu 11:00 H 2053

Nonequlibrium dynamics of s- and d-wave superconductors — •Holger Krull[2], Götz S. Uhrig[1], Andreas P. Schnyder[2], and Dirk Manske[2] — [1]TU Dortmund, Dortmund, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

We study the nonequilibrium dynamics of s- and d-wave superconductors, which are induced by a ultra-short pump pulse or a quench, respectively. The dynamics is studied by use of the density matrix formalism as well as by analytical calculation. We focus on the temporal evolution of the order parameter. For s-wave superconductors the nonadiabatic evolution of the order parameter is well established in the collisionless regime. It shows a $1/\sqrt{t}$ decaying oscillation, which can be interpreted as Higgs mode in a superconductor. Here, we consider the evolution of a d-wave order parameter and compare it with the s-wave case.

TT 86: Correlated Electrons: (General) Theory 2

Time: Thursday 9:30–13:00 Location: H 3005

TT 86.1 Thu 9:30 H 3005

A dual-fermion analysis of the Anderson-Hubbard model — •Patrick Haase[1], Shuxiang Yang[2], Thomas Pruschke[1], Juana Moreno[2], and Mark Jarrell[2] — [1]Georg-August Universität Göttingen — [2]Louisiana State University

We apply the recently-developed dual-fermion method for disordered interacting systems to the Anderson-Hubbard model. This method treats both disorder and interaction on equal footing, takes into account non-local correlations systematically, and thus represents a significant extension over the single-site mean-field description. We analyze the metal-insulator transition as well as the anti-ferromagnetic transition of the three-dimensional cubic lattice, by looking at both the one- and two-particle quantities, like the local Green function and the conductivity.

TT 86.2 Thu 9:45 H 3005

Antiferromagnetic phase transition in the Hubbard model from diagrammatic multi-scale perspective — •Daniel Hirschmeier[1], Hartmut Hafermann[2], Emanuel Gull[3], Alexander Lichtenstein[1], and Andrey Antipov[3] — [1]Universität Hamburg, I. Institut für Theoretische Physik, Hamburg, Deutschland — [2]University of Michigan, Ann Arbor, USA — [3]Institut de Physique Theorique (IPhT), Gif-sur-Yvette, France

We have studied the phase diagram of the antiferromagnetic transition of the Hubbard model in three dimensions, employing the ladder dual fermion approach. This diagrammatic extension of dynamical mean field theory embeds the non-local correlations into the problem and allowed us to extract universal, Heisenberg like critical exponents of the spin susceptibility and the correlation length for large and intermediate values of the Coulomb repulsion. This critical behaviour is coincident with the opening of a gap in the density of states, reflecting a relation between single- and two-particle quantities. Furthermore we discuss the impact of the gap in the density of states on the critical properties of the phase transition.

TT 86.3 Thu 10:00 H 3005

Gutzwiller variational wave function for a two-orbital Hubbard model on a square lattice — •Kevin zu Münster — Philipps University, Marburg, Germany

Gutzwiller variational wave functions can be evaluated exactly in infinite dimensions by the introduction of a gauge in the variational parameters. We present the generalization of this method for multiorbital systems and its application to a finite-dimensional lattice. We show numerical results for a two-dimensional Hubbard model with p_x-p_y symmetry. A variation of the underlying Fermi surface leads to features like Pomerantchuk instabilities or a change of the Fermi surface topology.

TT 86.4 Thu 10:15 H 3005

Interplay between Point-Group Symmetries and the Choice of the Bloch Basis in Multiband Models — •Stefan A. Maier[1] and Carsten Honerkamp[1,2] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52056 Aachen, Germany — [2]Member of JARA-FIT, Jülich-Aachen Research Alliance–Fundamentals of Future Information Technology

We analyze the point-group symmetries of generic multiband tight-binding models with respect to the transformation properties of the effective interactions. While the vertex functions in the orbital language may transform non-trivially under point-group operations, their point-group behavior in the band language can be simplified by choosing a suitable Bloch basis. We show that, for a large class of models, a natural Bloch basis exists, in which the vertex functions in the band language transform trivially under all point-group operations [cf. our article in *Symmetry*, **5(4)**, 313 (2013)]. As a consequence, the point-group symmetries can be used to reduce the computational effort in perturbative many-particle approaches, such as the functional renormalization group.

TT 86.5 Thu 10:30 H 3005

Towards high-performance functional renormalization group calculations for interacting fermions — •Julian Lichtenstein[1], Stefan A. Maier[1], Carsten Honerkamp[1,2], Edoardo Di Napoli[3], and Daniel Rohe[4] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [2]JARA-FIT, Jülich-Aachen Research Alliance–Fundamentals of Future Information Technology — [3]AICES, RWTH Aachen University, Germany — [4]Forschungszentrum Juelich GmbH, Juelich, Germany

We show that the flow equations of the singular-mode functional renormalization group (SM-FRG) approach put forward by Wang et al. [1] can be derived from an exchange parametrization of the two-fermion interaction [2] by introducing an additional approximation. Furthermore, we present a new variant of the SM-FRG, in which, unlike in the original variant, the interaction is represented in a unique way. We then discuss the applicability of the approximation made in addition to an exchange parametrization. Finally, we argue that the approximation made facilitates more efficient multiband calculations on a larger number of multi-core CPUs.

[1] Wang et al., *Phys. Rev. B* **85**, 035414 (2012).
[2] C. Husemann and M. Salmhofer, *Phys. Rev. B* **79**, 195125 (2009)

TT 86.6 Thu 10:45 H 3005

Summing parquet diagrams via the functional renormalization group: x-ray problem revisited[1] — •Philipp Lange, Casper Drukier, Anand Sharma, and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt

We present a simple and efficient method for summing so-called parquet diagrams of fermionic many-body systems with competing instabilities using the functional renormalization group. Our method is based on partial bosonization of the interaction using multi-channel Hubbard-Stratonovich transformations. A straightforward truncation of the resulting flow equations retaining only the frequency-independent parts of the two-point and three-point functions amounts to solving coupled Bethe-Salpeter equations for the effective interaction to leading logarithmic order. We apply our method to the x-ray problem and derive the singular frequency dependence of the x-ray response function and the particle-particle susceptibility. Our method can be applied to various other problems involving strong fluctuations in more than one scattering channel.

[1] G. D. Mahan, Phys. Rev. 163, 612 (1967).

TT 86.7 Thu 11:00 H 3005

Steps towards the application of two-particle irreducible functional renormalization group — •Jan Frederik Rentrop[1,2], Severin Georg Jakobs[1,2], and Volker Meden[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [2]JARA FIT - Fundamentals of Future Information Technology, 52056 Aachen, Germany

Functional renormalization group (RG) is an established method for the investigation of non-relativistic correlated quantum many-body problems in low dimensions. Commonly, the functional RG flow equations are derived in generating functional formalism and formulated for one-particle irreducible (1PI) vertex functions. However, generating functionals have long been written in a 2PI form as well. Based on these, proposals for 2PI functional RG schemes have been made. These mainly differ from one another with respect to the introduction of the flow parameter. It is remarkable that hardly any calculations for particular systems employing these proposed schemes have been published. Having performed toy model calculations for the quantum anharmonic oscillator, our recent work aims for a study of the single impurity Anderson model in equilibrium. The goal of this talk is to place 2PI schemes into a broader context (how they relate to other methods) and to present some data to evaluate the performance of the 2PI schemes in comparison to other schemes, in particular 1PI ones.

15 min. break.

TT 86.8 Thu 11:30 H 3005

From infinite to two dimensions through the functional renormalization group — •Ciro Taranto[1], Sabine Andergassen[2], Johannes Bauer[3], Karsten Held[1], Andrey Katanin[4], Walter Metzner[5], Georg Rohringer[1], and Alessandro Toschi[1] — [1]Institute for solid state physics, Vienna University of Technology, Austria — [2]Institute for theoretical physics and CQ center for collective quantum phenomena, University of Tübingen, Germany —

[3]Department of Physics, Harvard University, Usa — [4]Institute of metal Physics, Ural Federal University, Ekatrinburg, Russia — [5]Max Planck institute for Solid State research, Stuttgart, Germany

We present a novel scheme for an unbiased and non-perturbative treatment of strongly correlated fermions. The proposed approach combines two of the most successful many-body methods, i.e., the dynamical mean field theory (DMFT) and the functional renormalization group (fRG). Physically, this allows for a systematic inclusion of non-local correlations via the flow equations of the fRG, after the local correlations are taken into account non-perturbatively by the DMFT. To demonstrate the feasibility of the approach, we present numerical results for the two-dimensional Hubbard model at half-filling.

TT 86.9 Thu 11:45 H 3005

Correlated starting points for the functional renormalization group — •Nils Wentzell[1,2,3], Ciro Taranto[3], Andrey Katanin[4,5], Alessandro Toschi[3], and Sabine Andergassen[1,2] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — [2]Institut für Theoretische Physik and CQ Center for Collective Quantum Phenomena, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany — [3]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [4]Institute of Metal Physics, Kovalevskaya Str., 18, 620990, Ekaterinburg, Russia — [5]Ural Federal University, 620002, Ekaterinburg, Russia

We present a general frame to extend functional renormalization group (fRG) based computational schemes by using an exactly solvable *interacting* reference problem as starting point for the RG flow. The systematic expansion around this solution accounts for a non-perturbative inclusion of correlations. Introducing auxiliary fermionic fields by means of a Hubbard-Stratonovich transformation, we derive the flow equations for the auxiliary fields and determine the relation to the conventional weak-coupling truncation of the hierarchy of flow equations. As a specific example we consider the dynamical mean-field theory (DMFT) solution as reference system, and discuss the relation to the recently introduced DMF^{2}RG and the dual-fermion formalism.

TT 86.10 Thu 12:00 H 3005

The virial theorem within many-body extensions of density functional theory — •Andreas Östlin[1,2], Wilhelm Appelt[2,3], Liviu Chioncel[2,3], and Levente Vitos[1,4,5] — [1]Applied Materials Physics, Department of Materials Science and Engineering, KTH Royal Institute of Technology, Stockholm SE-100 44, Sweden — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [3]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [4]Department of Physics and Materials Science, Uppsala University, P.O. Box 516, SE-75120 Uppsala, Sweden — [5]Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Budapest H-1525, P.O. Box 49, Hungary

The virial theorem provides a relation between kinetic and potential energies for a large range of physical systems, and almost has the status of a conservation law. We investigate the fulfillment of the virial theorem for electronic structure calculations, in the framework of Density Functional Theory (DFT) both within the Local Density Approximation (LDA) and its Dynamical Mean Field Theory extension (LDA+DMFT). We demonstrate its validity for metals.

TT 86.11 Thu 12:15 H 3005

Quantum electrodynamical time-dependent density functional theory on a lattice — •Mehdi Farzanehpour[1] and Ilya Tokatly[1,2] — [1]Nano-Bio Spectroscopy group and ETSF Scientic Development Centre, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, E-20018 San Sebastian, Spain — [2]IKERBASQUE, Basque Foundation for Science, E-48011 Bilbao, Spain

We present a rigorous formulation of the time-dependent density functional theory for interacting lattice electrons strongly coupled to cavity photons. We start with an example of one particle on a Hubbard dimer coupled to a single photonic mode, which is equivalent to the single mode spin-boson model or the quantum Rabi model. For this system we prove that the electron-photon wave function is a unique functional of the electronic density and the expectation value of the photonic coordinate, provided the initial state and the density satisfy a set of well defined conditions. Then we generalize the formalism to many interacting electrons on a lattice coupled to multiple photonic modes and prove the general mapping theorem. We also show that for a system evolving from the ground state of a lattice Hamiltonian any density with a continuous second time derivative is locally v-representable.

TT 86.12 Thu 12:30 H 3005

Inverse Mean Field theories — •Peter Schmitteckert — Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

Methods based on many particle wave functions are naturally suited to describe strongly correlated quantum system and enable the description of non-perturbative problems. However, an intuitive description of many particle wave functions is often lacking. In contrast, mean field (MF) theories cannot treat interaction effects rigorously, but provide simple pictures within a single particle framework. In mean field theories one typically introduces a mean field decoupling of the Hamiltonian which is then solved within a single particle description. Here we go the other direction. We first solve for a many particle wave function, which is then used to construct a corresponding MF description. Specifically we discuss different strategies to construct a suitable mean field theory, which can then be used to discuss the physical problem. Finally we address the problem of describing time dependent phenomena of correlated quantum systems within an inverse MF description.

TT 86.13 Thu 12:45 H 3005

Reduced density matrix functional theory via a wave function based approach — •Robert Schade[1], Peter Bloechl[1], and Thomas Pruschke[2] — [1]Institute for Theoretical Physics, Clausthal University of Technology, Clausthal, Germany — [2]Institute for Theoretical Physics, University of Goettingen, Goettingen, Germany

We propose a new method for the calculation of the electronic and atomic structure of correlated electron systems based on reduced density matrix functional theory (rDMFT). The density matrix functional is evaluated on the fly using Levy's constrained search formalism. The present implementation rests on a local approximation of the interaction reminiscent to that of dynamical mean field theory (DMFT). This wave function based approach can be integrated into the existing DFT framework by making use of natural orbitals.

Financial support by the DFG Research Unit FOR 1346 "Dynamical Mean-Field Approach with Predictive Power for Strongly Correlated Materials" is gratefully acknowledged.

TT 87: Low-Dimensional Systems: Molecular Conductors (jointly with CPP, HL, MA, O)

Time: Thursday 9:30–11:00 Location: H 3010

TT 87.1 Thu 9:30 H 3010

Nature of the empty electronic states of TCNQ and their thermal evolution due to the CDW instability of TTF-TCNQ revealed by NEXAFS — •Alisa Chernenkaya[1], K. Medjanik[1,2], P. Nagel[3], M. Merz[3], S. Schuppler[3], E. Canadell[4], J.-P. Pouget[5], and G. Schönhense[1] — [1]JGU, Mainz, Germany — [2]MAX-lab, Lund, Sweden — [3]KIT, Karlsruhe, Germany — [4]ICMAB, Bellaterra, Spain — [5]Uni Paris-Sud, Orsay, France

The electronic structure of TTF-TCNQ was studied by near-edge x-ray absorption fine structure (NEXAFS) to detect a signature of the Peierls transition at 54 K [1]. All experimental unoccupied TCNQ orbitals predicted by first-principles calculations are clearly resolved, the $\sigma^*(\pi(a_g,\ b_3u))$ orbital was observed for the first time [2]. The temperature dependence of NEXAFS peak intensities gives evidence of a subtle modification of the electronic structure when the charge density wave (CDW) fluctuations develop as the Peierls transition of the TCNQ stacks is approached from higher temperatures. These changes are explained on the basis of the charge transfer, the shape of the lower empty TCNQ molecular orbitals and the deformation of TCNQ during the pre-transitional CDW fluctuations. Finally the data suggest that the internal stack deformation consisting in a substantial out of plane displacement of the central ring with respect to the cyano-groups allows to gain C-C bonding energy which helps the stabilization of the Peierls transition on the TCNQ stack.

[1] J.P. Pouget, Z. Kristallogr. 219, 711, 2004.
[2] A. Chernenkaya et al., EPJB, accepted.

TT 87.2 Thu 9:45 H 3010

Observation of charge localization and the charge ordering transition in $(TMTTF)_2AsF_6$ using NEXAFS — •Katerina Medjanik[1], Alisa Chernenkaya[2], Sergej Nepijko[2], Gunnar Öhrwall[1], Pascale Foury-Leylekian[3], Pere Alemany[4], Enric Canadell[5], Gerd Schönhense[2], and Jean-Paul Pouget[3] — [1]Lund University, MAX IV Laboratory, 22100 Lund, Sweden — [2]Institut für Physik, JOGU, 55099 Mainz, Germany — [3]Laboratoire de Laboratoire de Physique des Solides, Université Paris-Sud, 91405 Orsay, France — [4]IQTCUB, Universitat de Barcelona, 08028 Barcelona, Spain — [5]ICMAB-CSIC, 08193 Bellaterra, Spain

High-resolution near-edge X-ray absorption fine structure (NEXAFS) measurements at MAX II, Lund (beamline I1011 [1]) were performed on a $(TMTTF)_2AsF_6$ [2] single crystal upon cooling from room temperature to 90 K. Systematic shifts of different spectral features of the F 1s and S 2p signal by up to 0.8 eV to opposite sides on the photon-energy scale with respect to the spectra at room temperature have been detected. Most likely, the shift of the S 2p signal is connected with the breakdown of itinerant conductivity and loss of screening when entering the charge-localization regime.The appearance of a new F 1s pre-edge signal upon entry into the charge ordering (CO) phase at 90 K is a clear fingerprint of the reorganization of the anions in the layered material and changing in the dimerization of molecular orbitals with respect to room temperature.Project funded by DFG through SFB Transregio 49.

[1] I. A. Kowalik et al., J. Phys.: Conf. Ser. 211, 012030 (2010);
[2] M. de Souza et al., Physica B, 405, 92 (2010).

TT 87.3 Thu 10:00 H 3010

Low-Energy Excitations in the Quantum Spin Liquid κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ — •Andrej Pustogow[1], Elena Zhukova[2], Boris Gorshunov[2], Marko Pinteric[3,4], Silvia Tomic[4], John Schlueter[5], and Martin Dressel[1] — [1]1. Physikalisches Institut Universität Stuttgart — [2]Moscow Institute of Physics and Technology, Russia — [3]Faculty of Civil Engineering, Maribor, Slovenia — [4]Institut za fiziku, Zagreb, Croatia — [5]Argonne National Laboratory, USA

The suppression of long range magnetic order due to geometrical frustration gives rise to the quantum spin liquid state. Theoretical considerations predict enhanced absorption within the Mott gap caused by spinons, which results in a low-frequency power-law behaviour of the optical conductivity, i.e. for $\hbar\omega_c < J \approx 250K$. To verify this hypothesis, the optical conductivity of the spin liquid candidate κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ was measured, where the dimerized organic molecules are arranged on a triangular lattice. An extremely wide energy range from radio frequencies up to the near infrared ($10^{-13}eV - 1eV$) was covered by dielectric spectroscopy, THz absorption and optical reflectivity measurements. We could indeed identify a power-law behaviour $\sigma(\omega) \propto \omega^{\beta}$ where two distinct exponents β change from 0.9 to 1.7 at low temperatures, with the corresponding crossover scaling with temperature: $\hbar\omega_c \approx k_BT$. While our results agree well with $(ZnCu)_3\ (OD)_6\ (Cl)_2$, another spin liquid candidate, theory predicts exponents of 2 and 3.33, respectively. Hence, these experimental findings may motivate a refinement of the theoretical framework.

TT 87.4 Thu 10:15 H 3010

Mott criticality in organic charge-transfer salts κ-$(BEDT\text{-}TTF)_2X$ studied by thermal expansion under He-gas pressure — •E. Gati[1], R. S. Manna[1], U. Tutsch[1], B. Wolf[1], L. Bartosch[2], T. Sasaki[3], H. Schubert[1], J. A. Schlueter[4], and M. Lang[1] — [1]Physikalisches Institut, Goethe Uni, SFB/TR49, D-60438 Frankfurt — [2]Inst. für Theoretische Physik, Goethe Uni, D-60438 FfM — [3]IMR, Tohoku University, Sendai 980577, Japan — [4]Materials Science Division, National Laboratory, Argonne, Illinois 60439, USA

The Mott transition and the underlying universality class have been intensively studied in the past. The proposal of a hitherto unknown *unconventional* universality class for the quasi 2D organic charge-transfer salt κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Cl$ (κ-Cl) [1], based on resistivity measurements, has attracted particular interest. In this compound, the Mott transition can be accessed by chemical pressure or the application of very small hydrostatic pressures of 300 bar. We will present measurements of the thermal expansion of κ-Cl under ^{4}He-gas pressure [2], an unique technique, which provides a very sensitive tool to investigate critical phenomena [3,4], including effects of coupling of electrons to the crystal lattice [5]. A comparison of our results with theoretical predictions of a scaling theory [4] shows that the critical properties are incompatible with the proposed unconventional universality class.

[1] F. Kagawa et al., Nature 436, 534 (2005).
[2] R. S. Manna et al., Rev. Sci. Instrum. 83, 085111 (2012).
[3] M. de Souza et al., PRL 99, 0370031 (2007).
[4] L. Bartosch et al., PRL 104, 245701 (2010).
[5] M. Zacharias et al., PRL 109, 176401 (2012).

TT 87.5 Thu 10:30 H 3010

Electronic structure and superconductivity of multi-layered organic charge transfer salts — •Harald O. Jeschke, Michaela Altmeyer, Daniel Guterding, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt

We examine the electronic properties of polymorphs of $(BEDT\text{-}TTF)_2Ag(CF_3)_4(TCE)$ (1,1,2-trichloroethane) within density functional theory (DFT). While a phase with low superconducting transition temperature $T_c = 2.6$ K exhibits a κ packing motif, two high T_c phases are layered structures consisting of α' and κ packed layers. We determine the electronic structures and discuss the influence of the insulating α' layer on the conducting κ layer. In the κ-α'_1 dual-layered compound, we find that the stripes of high and low charge in the α' layer correspond to a stripe pattern of hopping parameters in the κ layer. Based on the different underlying Hamiltonians, we study the superconducting properties and try to explain the differences in T_c.

TT 87.6 Thu 10:45 H 3010

New Charge Transfer Systems based on PAHs — •Antonia Morherr[1], Sebastian Witt[1], Martin Baumgarten[2], Harald O. Jeschke[3], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe Universität Frankfurt, D-60438 Frankfurt am Main — [2]MPI für Polymerforschung, D-55128 Mainz — [3]Institut für Theoretische Physik, Goethe Universität Frankfurt, D-60438 Frankfurt am Main

The Polycyclic Aromatic Hydrocarbons (PAHs) Picene, Coronene and Phenanthrene attracted strong attention in the last years as first superconducting PAHs when intercalated with potassium [1]. K_3Picene shows a T_c of 18 K and the T_c of intercalated Coronene lies between 3.5 K and 15 K [2].
Here, we present charge transfer complexes with PAHs representing donor or acceptor molecules of these complexes. The knowledge of different crystallization modes of these systems, e.g. mixed stack or alternating stack configuration, are important for the physical proper-

ties. The complexes were grown by horizontal vapor growth technique or by growth from solution. Crystal structures, electrical transport measurements and spectroscopical investigations are presented in this contribution. In addition to the experimental data, we present band-structure calculations, which were performed by density functional methods. The interpretation of both is one approach to understand growing conditions of different stack configurations and an important step towards the design of new charge transfer complexes.

[1] R. Mitsuhashi et al., Nature 464, 76 (2010)
[2] Y. Kubozono et al., Phys. Chem. Chem. Phys. 13, 16476, (2012)

TT 88: Transport: Carbon Nanotubes

Time: Thursday 9:30–10:45 Location: A 053

TT 88.1 Thu 9:30 A 053

The excitation spectrum of a carbon nanotube — from 0 to 2 electrons — Daniel Schmid[1], Magdalena Marganska[2], Siddharth Buddhiraju[2], Peter Stiller[1], Alois Dirnaichner[1], Milena Grifoni[2], •Andreas K. Hüttel[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Defect- and contamination free, suspended single wall carbon nanotubes (CNTs) display a highly regular transport spectrum. The spectral features directly reflect the properties of the underlying graphene lattice, modified by curvature and finite length effects as well as the cylindrical topology of the nanotube.

We present and analyze data on the first two Coulomb blockade oscillations ($0 \leq N_{\mathrm{el}} \leq 2$) of such a system. Sharp differential conductance features enable the observation of multiple excited states of the trapped electronic system in variable angle magnetic fields. The analysis of the $N_{\mathrm{el}} = 1$ data provides us with direct knowledge of the single particle level spectrum. In contrast, the $N_{\mathrm{el}} = 2$ spectrum is dominated by the electron-electron interactions. In both regimes, the spectra are governed by the underlying symmetries of the CNT Hamiltonian.

Our model is based on a minimal one-shell Hamiltonian of a CNT with spin-orbit coupling and valley mixing and taking into account a magnetic field, extended to include two shells and the exchange interaction.

TT 88.2 Thu 9:45 A 053

Influence of spin-orbit interaction and chirality on Fabry-Perot interference in carbon nanotubes — •Alois Dirnaichner[1], Miriam del Valle[2], Karl Götz[1], Felix Schupp[1], Andreas K. Hüttel[1], Christoph Strunk[1], and Milena Grifoni[2] — [1]Institute of Experimental and Applied Physics, University of Regensburg — [2]Institute for Theoretical Physics, University of Regensburg

For highly transparent contact interfaces a carbon nanotube can be described as an electronic Fabry-Perot interferometer combining weak scattering at the contacts with a one-dimensional ballistic waveguide. In experiments on clean single wall carbon nanotubes we observe complex gate and bias voltage dependent interference patterns in conductance. This includes slow envelope beats as well as an apparent frequency doubling. Using an analytical scattering matrix model as well as numerical tight-binding calculations we show that such complex interference patterns can arise from the chirality and the spin-orbit interaction of a nanotube. Theoretical expectations for different types of nanotubes are compared with the experiment.

TT 88.3 Thu 10:00 A 053

Thermally induced subgap features in the cotunneling spectroscopy of a carbon nanotube — Sascha Ratz[1], •Andrea Donarini[1], Daniel Steininger[2], Thomas Geiger[2], Amit Kumar[2], Andreas Huettel[2], Christoph Strunk[2], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

We report on the nonlinear cotunneling spectroscopy of a carbon nanotube quantum dot coupled to Nb superconducting contacts [1]. Our measurements show rich subgap features in the stability diagram which become more pronounced as the temperature is increased. Subgap features in the tunnelling spectroscopy of hybrid superconductor-quantum dot structures are commonly attributed to Andreev reflection processes. However, applying a transport theory based on the Liouville-von Neumann equation for the density matrix, we show that, in the parameter range of our experiments, the subgap transport properties can be attributed solely to processes involving sequential as well as elastic and inelastic cotunneling of quasiparticles thermally excited across the gap. In particular, we predict thermal replicas of the elastic and inelastic cotunneling peaks, in agreement with our experimental results.

[1] S. Ratz, A. Donarini, D. Steininger et al. accepted by NJP, arXiv:1408.5000v2.

TT 88.4 Thu 10:15 A 053

Strong localization in defective carbon nanotubes — •Fabian Teichert[1,2], Andreas Zienert[2], Jörg Schuster[3], and Michael Schreiber[1] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Center for Microtechnologies, Technische Universität Chemnitz, Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

Carbon nanotubes (CNTs) are a prominent example for new materials in microelectronics, overcoming the miniaturization problem. So far CNTs cannot be grown or deposited in an ideal and reproducible way inside a device. As one consequence they contain defects.

The present work describes the transport properties of armchair CNTs with randomly positioned realistic defects, namely monovacancies and divacancies. The calculations are based on a fast, linearly scaling recursive Green's function formalism, allowing to treat large systems quantum-mechanically. The electronic structure is described by a density-functional-based tight-binding model.

The transmission spectrum of CNTs with single / many defects is studied. The influence of certain defect densities, the diameter of the CNT, and the temperature is investigated within a statistical analysis. It is shown that the system is in the regime of strong localization (i.e. Anderson localization), where the conductivity scales exponentially with the number of defects. This allows us to extract localization lengths, which depend on defect density, CNT diameter, and temperature. Finally, the correlation between the localization length and the single-defect conductance is shown.

TT 88.5 Thu 10:30 A 053

Random Telegraph Noise in Carbon Nanotubes — •Sung ho Jhang[1], Hyun-jong Chung[1], and Yung woo Park[2] — [1]Konkuk University, Seoul, Korea — [2]Seoul National University, Seoul, Korea

We have investigated random telegraph noise (RTN) observed in individual carbon nanotubes (CNTs). By analyzing the statistics and features of the RTN,we suggest that this noise originates from two different mechanisms; from the charge traps surrounding CNTs or from the random transition of defects within CNTs, activated by inelastic scattering with conduction electrons. The magnitude of resistance fluctuation is giant up to 60% of total resistance, much larger than inevitable thermal Nyquist noise. Due to the large RTN amplitude, the RTN approach could be developed into an effective probe to characterize single defects in CNTs. In addition, we show the RTN is sensitive to the encapsulated molecules inside CNTs, and report interacting noise behaviors.

TT 89: Transport: Quantum Dots, Quantum Wires, Point Contacts 1 (jointly with HL)

Time: Thursday 11:00–13:00 Location: A 053

TT 89.1 Thu 11:00 A 053

Interference of real and virtual transitions in quantum dot chains — •Fernando Gallego-Marcos, Rafael Sánchez, and Gloria Platero — Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain

We analyzed long-range transport through an ac driven triple quantum dot. Resonant transitions between separated and detuned dots are mediated by the exchange of n photons with the time-dependent field. An effective model is proposed in terms of higher-order transitions which involve the virtual only occupation of the intermediate dot [1]. The ac driving modulates the tunneling processes within the quantum dot system [2]. We investigate the interplay between real transitions through the centre dot and virtual long-range tunneling. We find configurations where the two paths interfere destructively and totally block the current. The effect of the driving phase will be emphasized.

[1] R. Sánchez, F. Gallego-Marcos, G. Platero,
Phys. Rev. B 89, 161402 (2014)
[2] F. Gallego-Marcos, R. Sánchez, G. Platero, arXiv:1408.4923

TT 89.2 Thu 11:15 A 053

Photon creation of a double quantum dot strongly coupled to the environment — •Michael Marthaler[1], Yasuhiro Utsumi[2], and Dmitri Golubev[3] — [1]Institut für Theoretische Festkörperphysik , Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]Department of Physics Engineering, Faculty of Engineering, Mie University, Japan — [3]O.V. Lounasmaa Laboratory, Aalto University School of Science, Finnland

We study a model which can describe a double quantum dot coupled to a transmission-line resonator. The charge eigenstates of the double dot couple strongly to the electromagnetic environment or phonons. We consider a situation where a transport voltage is applied and photons are created in the transmission-line resonator. Here we study the dependence of the average photon number in the resonator on the spectral function of the electromagnetic environment. We focus on three important cases, a strongly coupled environment with a small cut-off frequency, a structured environment peaked at a specific frequency and 1/f noise. We find that the electromagnetic environment can have a substantial impact on the photon creation. Resonance peaks are in general broadened and additional resonances can appear.

TT 89.3 Thu 11:30 A 053

Unconventional Superconductivity in Double Quantum Dots — Björn Sothmann[1], •Stephan Weiss[2], Michele Governale[3], and Jürgen König[2] — [1]Departement de Physique Theorique, Universite de Geneve, CH-1211 Geneve 4, Switzerland — [2]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [3]School of Physical and Chemical Sciences, Victoria University of Wellington, New Zealand

The formation of electron pairs is a prerequisite of superconductivity. The fermionic nature of electrons yields four classes of superconducting correlations with definite symmetry in spin, space and time. Here, we suggest double quantum dots coupled to conventional s-wave superconductors in the presence of inhomogeneous magnetic fields as a model system exhibiting unconventional pairing [1]. We propose two detection schemes for unconventional superconductivity, based on either Josephson or Andreev spectroscopy.

[1] B. Sothmann, S. Weiss, M. Governale, and J. König,
Phys. Rev. B **90**, 220501(R) (2014).

TT 89.4 Thu 11:45 A 053

Shot noise of a triple quantum dot transistor: Blurred polygons and enhancement at blockade — •Andreas Trottmann, Michael Niklas, Andrea Donarini, and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

A single-electron transistor model with triangular triple quantum dot as central element is studied by means of a Bloch-Redfield-type method with counting fields. Such a device is known to exhibit Coulomb as well as interference blockade due to the presence of orbital degeneracies [1]. Computed Fano factors follow a blurred polygonal pattern as function of the voltages, tend to behave oppositely as against average current, and are enhanced in certain blockade regions in particular. Expressions in an interference blockade region elucidate a counteraction between real and virtual transitions, a blocking condition, and a loss of purity. These effects can be captured describing the orbitally degenerate states based on a pseudospin within a Bloch sphere. Gate and bias thresholds in the Fano factor pattern reflect disparate connectivities, especially a lifting of an interference blockade due to the reachability of a second orbitally degenerate level in the latter case. Blurring is caused by the voltages dependence of axes and frequencies controlling the precession of the pseudospin.

[1] A. Donarini, G. Begemann, and M. Grifoni,
Phys. Rev. B 82, 125451 (2010).

TT 89.5 Thu 12:00 A 053

Circular-polarization-sensitive metamaterial based on triple quantum-dot molecules — •Panagiotis Kotetes[1], Pei-Qing Jin[2], Michael Marthaler[1], and Gerd Schön[1] — [1]Karlsruhe Institute of Technology — [2]Shanghai Maritime University

We propose a new type of chiral metamaterial based on an ensemble of artificial molecules formed by three identical quantum-dots in a triangular arrangement [1]. A static magnetic field oriented perpendicular to the plane breaks mirror symmetry, rendering the molecules sensitive to the circular polarization of light. By varying the orientation and magnitude of the magnetic field one can control the polarization and frequency of the emission spectrum. We identify a threshold frequency Ω, above which we find strong birefringence. In addition, Kerr rotation and circular-polarized lasing action can be implemented. We investigate the single-molecule lasing properties for different energy-level arrangements and demonstrate the possibility of circular polarization conversion. Finally, we analyze the effect of weak stray electric fields or deviations from the equilateral triangular geometry.

[1] P. Kotetes, P.-Q. Jin, M. Marthaler, and G. Schön, to appear in Phys. Rev. Lett. (arXiv:1406.6432).

TT 89.6 Thu 12:15 A 053

Electronic Transport through Cerium Nanocontacts — •Sebastian Kuntz[1], Oliver Berg[1], Christoph Sürgers[1], and Hilbert v. Löhneysen[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, D-76128 Karlsruhe — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, D-76021 Karlsruhe

We report on conductance measurements of Ce nanocontacts in mechanically controlled break-junctions (MCBJ) made from polycrystalline wires. The wires were cut from two different Ce ingots. One ingot was taken as-prepared after cooling from the melt and one ingot was carefully annealed over $\sim$ one week. We investigate the effect of cooling rate and γ-β-α-phase transformation on the conductance G of the nanocontacts measured at low temperatures. From a number of measurements of $G(\Delta x)$ where Δx is the distance between the two electrodes, we obtain conductance histograms. We focus on the conductance G^* of the "last plateau" before, with increasing Δx, G drops to zero. For Ce, different G^* values between 0.6 and 1.7 G_0 ($G_0 = 2e^2/h$) are observed, while for other rare-earth metals like Gd and Dy the last plateau occurs at $G^* \simeq 0.6$ G_0 and $G^* \simeq 0.9$ G_0, respectively. A possible explanation for the different G^* values of Ce is the additional contribution from the $4f$ state to the conductance whose distance from the Fermi level depends on the phase at low temperatures (α or β) and, hence, on the cooling rate of the sample.

TT 89.7 Thu 12:30 A 053

coherent single charge transport in MBE-grown InSb nanowire — •ning kang[1], sen li[1], dingxun fan[1], yuqing huang[1], libing wang[1], philippe caroff[2], and hongqi xu[1,2] — [1]Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, P. R. China. — [2]Solid State Physics, Lund University, Box 118, S-221 00 Lund, Sweden

InSb nanowire have unique properties, such as a narrow bandgap, strong spin-orbit interaction, large bulk mobility and a small effective mass. Here, we report fabrication and low-temperature electrical transport studies of InSb nanowires grown by MBE. Individual nanowire devices exhibit Coulomb blockade oscillations characteristic of single charge transport on length scales up to 700 nm. Detailed finite-bias transport measurements demonstrate coherent electron transport through discrete quantum levels. In the few electron regime, strong

signatures of higher order inelastic cotunneling occur which can directly be assigned to excited states. With this spectroscopy we extract the main characteristics of a single InSb nanowire, namely, the Lande factor and the the magnitude of the spin-orbit interaction. We also present initial experimental studies of devices composed of superconductor in proximity to single InSb nanowire. We observed gate-tunable supercurrent flowing through the InSb nanowire and multiple Andreev reflection characteristics. Our results demonstrate that the InSb nanowires can provide an ideal platform to exploring phase coherence quantum transport and topological electronics in a solid state system.

TT 89.8 Thu 12:45 A 053

Heat current as a tool to study quantum dot decay rates — •Jens Schulenborg[1], Roman Saptsov[2,3], Janine Splettstoesser[1], and Maarten R. Wegewijs[2,3,4] — [1]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Göteborg, Sweden — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]JARA - Future Information Technologies, Germany — [4]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany

Over the past years, potential applications in nanoelectronics, metrology and quantum information sparked great interest in studying the *dynamics* of time-dependently driven quantum dots. Recently, we investigated the decay rates of an interacting single-level quantum dot, weakly tunnel coupled to an electronic reservoir and brought out of equilibrium by a step pulse[1,2]. In particular, the *fermion-parity rate*[1] was found to be an additional time scale, besides the spin- and charge decay rate, of which the value is fundamentally restricted[2].

This work shows that the *time-dependent heat current* emitted from the dot gives new insights into the physics described by the fermion-parity rate. Using a master equation for the dot coupled to an electrode, we extract the decay rates and determine how they influence the decay of charge- and heat current. We find that, while the fermion-parity rate does not at all enter the charge current, it is the dominant time scale for the *dissipation of interaction energy* carried by the heat current.

[1] L. D. Contreras-Pulido et al., Phys. Rev. B **85**, 075301 (2012).
[2] R. Saptsov et al., Phys. Rev. B **90**, 045407 (2014).

TT 90: Low-Dimensional Systems: Topological Order 1 (jointly with DS, HL, MA, O)

Time: Thursday 11:30–13:00 Location: H 3010

TT 90.1 Thu 11:30 H 3010

Towards a complete characterization of 2d topological order using tensor networks and multipartite entanglement — •Roman Orus — Johannes-Gutenberg Universität, Mainz, Deutschland

Topological order in a 2d quantum matter can be determined by the topological contribution to the entanglement Renyi entropies. However, when close to a quantum phase transition, its calculation becomes cumbersome. In this talk I will show how topological phase transitions in 2d systems can be much better assessed by multipartite entanglement, as measured by the topological geometric entanglement of blocks. Specifically, I will present an efficient tensor network algorithm based on Projected Entangled Pair States (PEPS) to compute this quantity for a torus partitioned into cylinders, and then use this method to find sharp evidence of topological phase transitions in 2d systems with a string-tension perturbation. When compared to tensor network methods for Renyi entropies, this approach produces almost perfect accuracies close to criticality and, on top, is orders of magnitude faster. Moreover, I will show how the method also allows the identification of Minimally Entangled States (MES), thus providing a very efficient and accurate way of extracting the full topological information of a 2d quantum lattice model from the multipartite entanglement structure of its ground states.

TT 90.2 Thu 11:45 H 3010

Robustness of Symmetry Protected Topological Order in spin-2 quantum chains — •Augustine Kshetrimayum[1], Hong-Hao Tu[2], and Román Orús[1] — [1]Johannes Gutenberg University Mainz — [2]MPQ Munich

Topological order is a new kind of order that cannot be described using the Landau theory. It is associated to a non-local pattern of entanglement. When such non-local properties are protected by specific symmetries, it is known as Symmetry Protected Topological Order.

The existence of such a symmetry protected topologically ordered Intermediate Haldane phase for a spin-2 Heisenberg chain was suggested by Oshikawa in 1992. However, the evidence for its existence has remained quite elusive. More recently, it has been proven that such a phase exists in a family of generalized spin-2 quantum Heisenberg chains.

In this work, we study the robustness of this phase for generalized spin-2 quantum Heisenberg chains with uni-axial anisotropy, and in the thermodynamic limit. We find very robust symmetry-protected topologically ordered SO(5)-Haldane and Intermediate-Haldane phases, which we assess by a variety of methods including the entanglement spectrum of the system and the behavior of string-order parameters. Moreover, we study time-evolution properties of these phases. Our numerical results are based on using Matrix Product States (MPS) to represent the wave function, in combination with the infinite Time-Evolving Block Decimation (iTEBD) method.

TT 90.3 Thu 12:00 H 3010

Wire deconstructionism of two-dimensional topological phases — •Ronny Thomale[1], Titus Neupert[2], Claudio Chamon[3], and Christopher Mudry[4] — [1]Institut für Theoretische Physik, Universität Würzburg, Germany — [2]Princeton University, USA — [3]Boston University, USA — [4]PSI Zürich, Switzerland

A scheme is proposed to construct integer and fractional topological quantum states of fermions in two spatial dimensions. We devise models for such states by coupling wires of non-chiral Luttinger liquids of electrons, that are arranged in a periodic array. Which inter-wire couplings are allowed is dictated by symmetry and the compatibility criterion that they can simultaneously acquire a finite expectation value, opening a spectral gap between the ground state(s) and all excited states in the bulk. First, with these criteria at hand, we reproduce the tenfold classification table of integer topological insulators, where their stability against interactions becomes immediately transparent in the Luttinger liquid description. Second, we construct an example of a strongly interacting fermionic topological phase of matter with short-range entanglement that lies outside of the tenfold classification. Third, we expand the table to long-range entangled topological phases with intrinsic topological order and fractional excitations.

TT 90.4 Thu 12:15 H 3010

Symmetry Protected Phases in Geometrically Frustrated 1D Antiferromagnets — •Alexander Nietner, Emil J. Bergholtz, and Jens Eisert — Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany

Geometrically frustrated (GF) systems admit an exotic phenomenology, such as spin liquid states, which lack any local order parameter. To reach a better understanding of such behaviour we realize the spin one Heisenberg antiferromagnetic Δ-chain (HAD) as a simple GF system in a numerically feasible regime. Inspired by a projected entangled pairs picture, we relate this system to a double layered ferromagnetically coupled $s = 1/2$ HAD. We use the time dependent variational principle to compute the ground states of these systems and investigate their phase diagramme in the thermodynamic limit, analysing the entanglement spectra and the projective representations of the symmetry groups. Despite the simplicity of these systems, we find evidence of a topological phase transition for the latter one from the trivial phase in the weak ferromagnetic limit towards a symmetry protected nontrivial phase for a finite coupling strength. This is in good agreement with the fact that the corresponding $s = 1$ system is found to be in the topological Haldane phase.

TT 90.5 Thu 12:30 H 3010

Route to Topological Superconductivity via Magnetic Field Rotation — •Florian Loder, Arno P. Kampf, and Thilo Kopp — Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany

Apart from the very few spin-triplet superconductors with p-wave pairing symmetry, a candidate system for topological superconductivity is a conventional, two-dimensional s-wave superconductor in a magnetic field with a sufficiently strong Rashba spin-orbit coupling. Typically, the required magnetic field to convert the superconductor into a topologically non-trivial state is however by far larger than the upper critical field H_{c2}, which excludes its realization. Here we argue that this problem is overcome by rotating the magnetic field into the superconducting plane. We explore the topological transitions which occur upon changing the strength and the orientation of the magnetic field and show that an unusual superconducting state with finite-momentum pairing exists, which preserves its topological nature up to an in-plane field orientation. We discuss the realizability of this state at the superconducting interface between $LaAlO_3$ and $SrTiO_3$.

TT 90.6 Thu 12:45 H 3010

Topological phases of a chain of twist defects — •Abhishek Roy[1], Xiao Chen[2], and Jeffrey Teo[3] — [1]Institute of Theoretical Physics, University of Cologne, Koeln, Germany — [2]Department of Physics, University of Illinois at Urbana-Champaign, USA — [3]Department of Physics, University of Virgina, USA

A twist defect acts on a system of abelian anyons by permuting anyon labels in a manner that preserves their braiding properties.

We investigate a one dimensional chain of twist defects. The Hamiltonian consists of Wilson loop operators, each enclosing a pair of neighbouring defects. We explore both gapped and gapless phases. For the former, we use anyon pumping to classify the ground states. For the latter, we present mappings to known critical models.

We extend the above results from twofold defects (which are similar to Z_k parafermions) to threefold defects introduced by us earlier in an exactly solvable lattice model [1].

[1] J. C.Y. Teo, A. Roy, X. Chen. Phys. Rev. B 90, 115118

TT 91: Superconductivity: (General) Theory 1

Time: Thursday 11:30–13:00 Location: H 2053

TT 91.1 Thu 11:30 H 2053

***Ab initio* study of the interplay between superconductivity and magnetic fields in MgB_2** — •Alexandros Aperis, Pablo Maldonado, and Peter M. Oppeneer — Uppsala University, Uppsala, Sweden

Among the bulk superconductors broadly accepted to be mediated by phonons, MgB_2 exhibits a record high critical temperature of $T_c = 39$ K. The relatively simple crystal structure of this material makes it an ideal platform to investigate fundamental phenomena, such as the interplay between superconductivity and the Zeeman effect, at the *ab initio* level. Here we combine DFT calculations providing electronic band and phonon dispersions with numerical solutions of the fully anisotropic Eliashberg equations, to provide a complete picture of the modification of the two-band superconductivity in this compound at finite external magnetic fields and temperature. We predict interesting signatures in the $H-T$ phase diagram which could be experimentally probed.

TT 91.2 Thu 11:45 H 2053

Superconductivity in Metal-intercalated Dodecaborides — •Lilia Boeri[1] and Matteo Calandra[2] — [1]ITP-CP TU Graz, Petersgasse 16, 8010 Graz (Austria) — [2]IMPMC, UMR CNRS 7590, Sorbonne Universités - UPMC Univ. Paris 06, MNHN, IRD, 4 Place Jussieu, F-75005 Paris, France

Metal-Intercalated dodecaborides (MB_{12}) display different low-temperature behaviour depending on the nature of the metal atom M [1]. In this work, we employ a method based on real-space (Wannier) interpolation of phonon and electronic wave functions [2], to study from first-principles the fully anisotropic Migdal-Eliashberg of compounds with M=Zr, Sc and Lu, which are superconducting with critical temperatures of 5.82 , 0.39 and 0.48 K respectively. These compounds have long been conventional considered BCS-like superconductors, but recent recent optical and ARPES experiments displayed several anomalies, which were attributed to the presence of localized phonon modes and possible strong correlation effects [3,4].

[1] B.T. Matthias et al., Science **159**, 530 (1968).
[2] M. Calandra, G. Profeta, and F. Mauri,
Phys. Rev. B **82**, 165111 (2010).
[3] S. Thakur et al., Scientific Reports **3**, 3342 (2013).
[4] J. Teyssier et al., Phys. Rev. B **75**, 134503 (2007).

TT 91.3 Thu 12:00 H 2053

Charge Order in Cuprate Superconductors — •Sinan Bulut[1], Arno P. Kampf[1], and Bill A. Atkinson[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Augsburg, Germany — [2]Department of Physics and Astronomy, Trent University, Peterborough Ontario, Canada

Motivated by widespread experimental evidence of charge orders in underdoped cuprate superconductors, we study a three band model of a cuprate plane. Our calculations start from a pseudogap-like normal system with a reconstructed Fermi surface, and we search for charge instabilities. From the charge susceptibilities, we identify a charge ordering instability with an ordering wavevector, $\mathbf{q}^*$, that matches experimental results not only with respect to the doping dependence but more importantly regarding its magnitude and direction. Namely, $\mathbf{q}^*$ points *along the Brillouin zone axes*. Thus, our results clarify the discrepancy between many recent theoretical calculations and the experiments. We extend this calculation towards possible loop current instabilities and the charge ordering pattern in bilayer systems.

TT 91.4 Thu 12:15 H 2053

Resonant inelastic X-ray scattering of high-T_C cuprates — •Yi Lu[1] and Maurits W. Haverkort[2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]Max Planck Institute for Chemical Physics of Solids, Dresden

We present a systematic study of resonant inelastic X-ray scattering (RIXS) of high-T_c superconducting cuprates using a single-band model. We show how the RIXS spectra evolve in metals, correlated metals and Mott insulators in the framework of dynamical mean-field theory using a recently developed impurity solver. In light of recent experiments, the dependence of RIXS cross-section on doping and incident photon energy were specifically investigated. Our work clarifies the debated interpretation of RIXS as a measurement of magnetic collective mode or simply incoherent excitations of the particle-hole continuum.

TT 91.5 Thu 12:30 H 2053

Critical analysis of the preformed pair physics: the attractive Hubbard model under a paring forcing field — •Agnese Tagliavini[1], Massimo Capone[2], and Alessandro Toschi[1] — [1]Institute for Solid State Physics, Vienna University of Technology, 1040 Wien, Austria — [2]Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy

The nature of the pseudogap features observed in correlated materials and its relation with superconductivity is still controversially debated. From the theoretical point of view, a new insight on the underlying physics can be obtained by studying the superconducting response to an external pairing field.

To this aim we consider the attractive Hubbard model where a preformed pair physics is realized in the strong-coupling limit: By means of Dynamical Mean-Field Theory, we study the superconducting response of the model to a static external pairing field (both uniform and local) focusing on the energetics.

We also compare our results with those obtained in the 2D repulsive Hubbard model, which is usually considered the basic model for high-Tc superconductors, where studies with cluster extensions of Dynamical Mean-Field Theory indicate the lack of preformed pairs.

TT 91.6 Thu 12:45 H 2053

Asymmetric Bethe-Salpeter equation for pairing and condensation — •Klaus Morawetz[1,2,3] and Pavel Lipavsky[4] — [1]Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics (IIP)Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — [3]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Ger-

many — [4]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

The Martin-Schwinger hierarchy of correlations is reexamined to derive the recently proposed asymmetric Bethe-Salpeter equation avoiding unphysical repeated collisions. Exceeding the parquet approximation an asymmetry appears in the selfconsistent propagators. This form is superior over the symmetric selfconsistent one since it provides the Nambu-Gorkov equations and gap equation for fermions and the Beliaev equations for bosons without the use of anomalous propagators. The T-matrix with multiple scattering corrections allows to describe superconductivity above and below the critical temperature by the same theoretical footing and provides e.g. a critical velocity of pair excitation larger than the critical velocity of pair breaking in agreement with the experiments.

[1] B. Sopik, P. Lipavský, M. Männel, K. Morawetz, P. Matlock, Phys. Rev. B 84 (2011) 094529.
[2] K. Morawetz, J. Stat. Phys. 143 (2011) 482-500.
[3] P. Lipavský, K. Morawetz, B. Sopik, M. Männel, Eur. Phys. J. B 87 (2013) 8-1-10.

TT 92: Topological Insulators I (jointly with MA, DS, HL, O)

Time: Thursday 9:30–12:00 Location: EB 202

TT 92.1 Thu 9:30 EB 202

DETECTION OF SURFACE SPIN CURRENT IN 3-DIMENSIONAL TOPOLOGICAL INSULATOR, BiSbTeSe — •Masashi Shiraishi[1], Yuichiro Ando[1], Takahiro Hamasaki[1], Kohji Segawa[2], Satoshi Sasaki[2], Feng Yang[2], Mario Novak[2], and Yoichi Ando[2] — [1]Kyoto Univ., Japan — [2]ISIR, Osaka Univ., Japan

Topological insulators (TIs) attract tremendous attention in recent years, since topologically-protected edge current is a persistent pure spin current. The first detection of the edge current was achieved by using 2-dimensional TI, HgTe quantum well [1], and the next challenge is to detect the edge current in 3-dimensional TIs, because a number of spin channel can be dramatically increased. Whereas Li et al. claimed that they successfully detected the surface spin current in Bi2Se3 by using an electrical spin accumulation method [2], the polarity of the spin signals is not accordance with the direction of magnetization of a detector ferromagnet. Thus, there is still open for discussion how to detect the edge spin current. Here, we present the detection of the edge spin current of BiSbTeSe, which is a bulk insulative TI [3]. The spin signal due to the spin accumulation was detected electrically, and was observed up to 150 K [4].

[1] M. Koenig et al., Science 318, 766 (2007). [2] C. Li et al., Nature Nanotech. 9, 218 (2014). [3] T. Arakane, Yo. Ando et al., Nature Commun. 3, 636 (2011). [4] Yu. Ando, M. Shiraishi et al., Nano Lett., in press.

TT 92.2 Thu 9:45 EB 202

First-principles calculation of quasiparticle spin interference and scattering processes on 3D topological insulators — •Philipp Rüssmann, Phivos Mavropoulos, Nguyen H. Long, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We present density-functional calculations of the quasiparticle interference (QPI) due to scattering of electrons off magnetic and non-magnetic impurities at the surface of the strong topological insulator Bi_2Te_3. The focus of our work is the calculation and analysis of possible spin-dependent scattering processes and their relation to the QPI pattern observed in experiment. The presence of an impurity magnetic moment leads to broken time-reversal symmetry and the protection against back-scattering is lifted. Therefore, we investigate magnetic transition-metal adatoms as well as non-magnetic Bi and Te adatoms on Bi_2Te_3. Finally, we compare the QPI pattern and scattering processes at different energies around the Fermi energy and discuss the importance of the hexagonal warping of the constant energy contours.

The electronic structure calculations are carried out with our KKR-Green function method for scattering properties at defects [1]. We acknowledge financial support from the DFG (SPP-1666), from the VITI project of the Helmholtz Association and computational support from the JARA-HPC Centre at the RWTH Aachen University.

[1] N. H. Long, P. Mavropoulos, B. Zimmermann, D. S. G. Bauer, S. Blügel, and Y. Mokrousov, Phys. Rev. B **90**, 064406 (2014).

TT 92.3 Thu 10:00 EB 202

Momentum resolved spin dynamics of bulk and surface excited states in the topological insulator Bi_2Se_3 — C Cacho[1], A Crepaldi[2], M Battiato[3], J Braun[5], H Ebert[5], K Hricovini[4], •Jan Minar[5,6], and F Parmigiani[2] — [1]Central Laser Facility, STFC Rutherford Appleton Laboratory, Harwell, United Kingdom — [2]Elettra - Sincrotrone Trieste, Italy — [3]Institute of Solid State Physics, Vienna University of Technology — [4]Universite de Cergy-Pontoise, France — [5]LMU München, Germany — [6]University of West Bohemia, Plzen, Czech Rep.

The prospective of optically inducing a spin polarized current for spintronic devices has generated a vast interest in the out-of-equilibrium electronic and spin structure of topological insulators (TIs). In this presentation we prove that only by measuring the spin intensity signal over several order of magnitude in spin, time and angle resolved photoemission spectroscopy (STAR-PES) experiments is it possible to comprehensively describe the optically excited electronic states in TIs materials. The experiments performed on Bi2Se3 reveal the existence of a Surface-Resonance-State in the 2nd bulk band gap interpreted on the basis of fully relativistic ab-initio spin resolved photoemission calculations. Remarkably, the spin dependent relaxation of the hot carriers is well reproduced by a spin dynamics model considering two non-interacting electronic systems, derived from the excited surface and bulk states, with different electronic temperatures. For more details see: Cacho et all.,
http://arxiv.org/abs/1409.5018

TT 92.4 Thu 10:15 EB 202

Spin structure of the Dirac state of the topological insulator Bi_2Te_3(0001) — •Christoph Seibel[1], Henriette Maass[1], Hendrik Bentmann[1], Jürgen Braun[2], Jan Minár[2], Taichi Okuda[3], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Department Chemie, Physikalische Chemie, Universität München, Butenandtstrasse 5-13, D-81337 München — [3]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

Three-dimensional topological insulators feature non-trivial surface states in the fundamental band gap of the bulk. In particular, the spin texture of these topological surface states (TSS) attracts attention in the context of possible applications in spintronics. We have performed angle- and spin-resolved photoemission measurements to analyze the three-dimensional spin texture of the TSS of the topological insulator Bi_2Te_3. The measured photoelectron spin-polarization is found to significantly deviate from the anticipated ground-state spin texture of the TSS, as derived e.g. on the basis of first-principles calculations. Possible origins of our observations are discussed in terms of the influence of spin-orbit coupling on the photoemission process. We compare our experimental data to the results of fully relativistic one-step photoemission calculations.

TT 92.5 Thu 10:30 EB 202

Atomic relaxations in Bi_2Se_3 (0001) — Sumalay Roy[1], •Holger L. Meyerheim[1], Katayoon Mohseni[1], Arthur Ernst[1], Mikhail Otrokov[2,3], Maia G. Vergniory[1,2], Gregor Mussler[4], Christian Tusche[1], Evgueni Chulkov[2,3], and Jürgen Kirschner[1,5] — [1]MPI f. Mikrostrukturphysik, D-06120 Halle, Germany — [2]DIPC, San Sebastian, Spain — [3]Tomsk St. Univ. , Russia — [4]FZ Jülich, Germany — [5]MLU Halle-Wittenberg, Germany

Surface x-ray diffraction analysis of the Bi_2Se_3(0001) surface reveals an expansion of the top Se-Bi interlayer spacing in the range between 2 and 17% relative to the bulk. It is directly related to the concentration of surface contaminants like carbon and is observed in both, single crystals and MBE grown ultrathin films. Deeper layers and the first van der Waals gap remain unrelaxed. Ab-initio calculations which are in agreement with angular resolved photoemission experiments reveal

that carbon acts as an n-dopant, while the top layer expansion induces a shift of the Dirac point towards the bulk conduction band of Bi_2Se_3 [1,2].

[1] S. Roy, H.L. Meyerheim, A. Ernst et al., PRL **113**, 116802 (2014);
[2] S. Roy, H.L. Meyerheim, K. Mohseni et al., PRB **90**, 155456 (2014)

This work is supported by SPP1666 (Topological Insulators) of the DFG.

TT 92.6 Thu 10:45 EB 202

Spin resolved momentum microscopy of the topological insulator Bi_2Se_3 — •Christian Tusche[1], Martin Ellguth[1], Shigemasa Suga[1,2], Holger L. Meyerheim[1], and Jürgen Kirschner[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Institute of Scientific and Industrial Research, Osaka, Japan — [3]Institut für Physik, Martin-Luther-Universität, Halle, Germany

Topological insulators are a new class of materials that attracted wide interest by their electronic structure with unusual relations of electron spin and momentum, leading to highly spin polarized "Dirac-cone" surface states. Recently, comprehensive experimental access to such band structures became feasible by spin resolved momentum microscopy. This novel concept combines high resolution imaging of photoelectrons in two-dimensional (k_x, k_y) sections with a highly efficient imaging spin filter. Electron reflection at a Au/Ir(100) mirror allows us to measure 5000 spin-resolved points in the surface Brillouin zone, simultaneously.

We show that the band-structure of Bi_2Se_3 is characterized by highly spin polarized states within the complete Brillouin zone, beyond the "Dirac cone" surface state. For the latter we find that the spin polarization of photoelectrons can reach up to 90%, the highest value reported so far. A direct conclusion on the ground state polarization in these systems is complicated by the peculiar interplay between spin- and light-polarization in the photoemission, as directly observed in spin-resolved (k_x, k_y) images.

This work is supported by SPP1666 (Topological Insulators) of the DFG. M.E. acknowledges support by the BMBF (05K12EF1).

TT 92.7 Thu 11:00 EB 202

The magnetism of Ni adatoms adsorbed on the TI Bi_2Te_2Se — Jan Honolka[1], Martin Vondráček[1], •Lasse Cornils[2], Malte Schüler[3], Markus Dunst[4], Jonas Warmuth[2], Lihui Zhou[2], Anand Kamlapure[2], Alexander Ako Khajetoorians[2,5], Matteo Michiardi[6], Lucas Barreto[6], Philip Hofmann[6], Jian-Li Mi[6], Martin Bremholm[6], Bo B. Iversen[6], Cinthia Piamonteze[7], Hubert Ebert[4], Jan Minar[4,8], Tim Wehling[3], Roland Wiesendanger[2], and Jens Wiebe[2] — [1]Inst. of Physics ASCR, Prague, Czech Republic — [2]INF, University of Hamburg, Germany — [3]Inst. of Theo. Physics, University of Bremen, Germany — [4]LMU München, Germany — [5]IMM, Radboud University Nijmegen, The Netherlands — [6]iNano, Aarhus University, Denmark — [7]PSI, Switzerland — [8]New Technologies-Research Center, University of West Bohemia, Pilsen, Czech Republic

The predicted gap opening in the surface state of topological insulators (TIs) induced by surface magnetic doping, and the associated novel electron phases, have recently caught strong interest of the scientific community. However, the experimental evidence of an induced gap opening is still controversial [1] and calls for a detailed investigation of the magnetism of different adatoms. Here, we show by a combined XMCD, ARPES and STS study, that Ni adatoms on the TI Bi_2Te_2Se reveal a surprising behaviour: While there is no detectable XMCD signal at the Ni $L_{2,3}$-edges, the XAS spectrum unveils a considerable resonant absorption of the d-shell. The results are analyzed by *ab-initio* calculations. [1] J. Honolka *et al.*, PRL **108**, 256811 (2012).

TT 92.8 Thu 11:15 EB 202

Fe-induced stress on Bi_2Se_3(0001) — •Kenia Novakoski Fischer, Safia Ouazi, Dirk Sander, and Jürgen Kirschner — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle

The topological insulator Bi_2Se_3 has attracted intense research activity since its discovery 5 years ago [1]. Here we present the first experimental study of the stress change induced by sub-monolayer deposition of Fe on Bi_2Se_3. Deposition of 0.2 ML Fe at 300 K induces a stress change of -2.3 N/m. On the contrary, deposition of Fe at 150 K leads to negligible stress change of less than -0.2 N/m. The growth of Fe at 473 K induces a stress of -3.4 N/m. LEED reveals that the hexagonal diffraction pattern of the substrate gets blurred for deposition at 150 K, whereas deposition at higher temperature induces faint diffraction spots indicative of precursor of possible FeSe formation. We discuss these results in view of a recent STM study [2], where the authors suggest thermally activated sub-surface doping of Bi_2Se_3 by Fe.

[1] H. Zhang, C.X. Liu, X.L. Qi, X. Dai, Z. Fang, and S. C. Zhang, Nat. Phys. 5 (2009) 438; W. Zhang, R. Yu, H.J. Zhang, X. Dai, and Z. Fang, New Journal of Physics 12 (2010) 065013. [2] T. Schlenk, M. Bianchi, M. Koleini, A. Eich, O. Pietzsch, T. O. Wehling, T. Frauenheim, A. Balatsky, J.-L. Mi, B. B. Iversen, J. Wiebe, A. A. Khajetoorians, Ph. Hofmann, and R. Wiesendanger, Phys. Rev. Lett. 110 (2013) 126804

TT 92.9 Thu 11:30 EB 202

Atomic structure and magnetism of Fe on Bi_2Se_3 — •Andrey Polyakov[1], Holger L. Meyerheim[1], E. Daryl Crozier[2], Robert A. Gordon[3], Maia G. Vergniory[4], Arthur Ernst[1], Evgueni V. Chulkov[4], and Jürgen Kirschner[1,5] — [1]MPI f. Mikrostrukturphysik, D-06120 Halle, Germany — [2]SFU, Burnaby, V5A 1S6 BC, Canada — [3]CLS at APS Sector 20, Argonne, IL, USA — [4]DIPC, San Sebastian, Spain — [5]MLU Halle-Wittenberg, Germany

We have carried out extended x-ray absorption fine structure (EXAFS) and surface x-ray diffraction (SXRD) experiments in combination with ab-initio calculations to investigate the geometric and magnetic properties of iron deposited on the (0001) surface of the topological insulator Bi_2Se_3 in the coverage range between about 0.2 and 1.5 monolayers (ML). For iron deposited at T=170 K in the low coverage limit no polarization dependence of the EXAFS amplitude (electric field vector parallel vs. perpendicular to the surface of the bulk crystal) could be observed. In combination with the nearest neighbor distance of 2.42 Å this suggests that Fe atoms substitute bismuth atoms involving a local relaxation of the neighboring selenium atoms. Ab-initio calculations support this structural model and predict antiferromagnetic ordering of iron [1]. SXRD data collected at 1.5 ML indicate that iron atoms also occupy threefold hollow surface sites. Mild annealing leads to the formation of a bulk FeSe like structure. [1] M. G. Vergniory et al. PRB 89, 165202 (2014); This work is supported by SPP 1666 (Topological Insulators). Work at APS sector 20 is supported by the CLS and by US DOE under Contract No. DE-AC02-06CH11357

TT 92.10 Thu 11:45 EB 202

Signatures of Dirac fermion-mediated magnetic order — •Paolo Sessi[1], Felix Reis[1], Thomas Bathon[1], Konstantin Kokh[2], Oleg Tereshchenko[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Novosibirsk State University, 630090 Novosibirsk, Russia

The spin-momentum locking of topological states offers an ideal platform to explore novel magneto-electric effects. These intimately depend on the ability to manipulate the spin texture in a controlled way. Although numerous studies aimed to shed light on the role played by magnetic perturbations, contradictory results have been obtained and a clear picture is still missing. The interaction of surface magnetic moments with topological states has predominantly been performed by using spatial averaging techniques such as angle-resolved photoemission spectroscopy and x-ray magnetic circular dichroism. Here, we combine low-temperature scanning tunneling microscopy with single-adatom deposition to directly map the evolution of the electronic properties of topological states under the influence of different magnetic perturbations. By analyzing energy-resolved quasi-particle interfer- ence maps, we reveal signatures of Dirac fermion-mediated surface magnetic order for extremely dilute adatom concentrations. By using different magnetic elements and coverages, we find that this striking observation crucially depends on two parameters: single adatoms mag- netic anisotropy direction and energy-level alignment [1].

[1] P. Sessi et al., Nature Comm. 5, 5349 (2014).

TT 93: Graphen (organized by DS)

Time: Thursday 9:30–13:00 Location: H 0111

TT 93.1 Thu 9:30 H 0111

Graphene Growth and Isotope Engineering — •Michael Hilke[1,2], Eric Whiteway[1], Wayne Yang[1], and Victor Yu[1] — [1]McGill University, Montreal, Kanada — [2]FU Berlin, Berlin, Deutschland

Graphene is grown by chemical vapor deposition (CVD) on copper using different relative concentrations of C12 and C13 isotopes. This allows us to measure the dynamics of the growth and extract important growth parameters, in particular in relation to regular and fractal graphene (graphlocons) growth. Further, the use of different isotopes, opens the door to new phonon properties such as phonon Anderson localization, phonon waveguides and more generally phonon engineering.

TT 93.2 Thu 9:45 H 0111

Synthesis of long- range ordered crystalline Graphene by chemical vapor deposition over Iridium (111) films on Sapphire — •Arti Dangwal Pandey and Andreas Stierle — Deutsches Elektronen-Synchrotron, Hamburg, Germany

High-quality and large-area Graphene is in demand to exploit its unique physical properties for various applications, including future electronic devices and sensors. Large-area epitaxial graphene have been deposited successfully by CVD on transition metal single crystals. These substrates are of high quality, but very expensive. This drives the search for other alternatives to use cheaper substrates. Ir has low carbon solubility, and so Ir thin film is a good choice for growing Graphene on it. Only single article is published till date for preparing epitaxial graphene on single crystal Ir film. [1] We have synthesized long-range ordered crystalline Graphene over few nanometer thick Ir films deposited on sapphire. Ethylene is used as a carbon source for depositing graphene by CVD and Ir films are grown by physical vapor deposition. LEED reveals the long-range crystallinity of graphene and Ir films, and XPS measurements confirmed the high purity of Ir films. Influence of growth parameters on the quality of Ir film, and thus on Graphene, will be discussed in Detail.

[1] Chi Vo-Van et al. App. Phys. Lett. 98 (2011) 181903.

TT 93.3 Thu 10:00 H 0111

Rotated domain network in graphene on cubic-SiC(001) — •Victor Aristov[1,2,3], Alexander Chaika[1,4], Olga Molodtsova[2], Alexei Zakharov[5], Dmitry Marchenko[6], Jaime Sánchez-Barriga[6], Andrei Varykhalov[6], Sergey Babenkov[2], Marc Portail[7], Marcin Zielinski[8], Barry Murphy[4], Sergey Krasnikov[4], Olaf Luebben[4], and Igor Shvets[4] — [1]ISSP RAS Chengolovka, Russia — [2]DESY Hamburg, Germany — [3]Uni Hamburg, Germany — [4]Trinity College Dublin, Ireland — [5]MAX-lab Lund, Sweden — [6]BESSY Berlin, Germany — [7]CNRS-CRHEA Valbonne, France — [8]NOVASiC Le Bourget du Lac, France

The atomic structure of the cubic-SiC(001) surface during UHV graphene synthesis has been studied using PES, STM and LEED. The studies prove the synthesis of a uniform, millimeter-scale graphene overlayer consisting of nanodomains rotated by *13.5o relative to the <110>-directed boundaries. The preferential directions of the domain boundaries coincide with the directions of carbon atomic chains on the SiC(001)-c(2x2) reconstruction, fabricated prior to graphene synthesis. The presented data show the correlation between the atomic structures of the SiC(001)-c(2x2) surface and the graphene /SiC(001) rotated domain network and pave the way for optimizing large area graphene synthesis on low cost cubic SiC(001)/Si(001) wafers. Acknowledgments: This work was supported by the RAS, RFBR grants No 140200949 and 140201234, by the BMBF-Project No. 05K12GU2, PSP-Element No. U4606BMB1211, by a Marie Curie IIF grant No 12/IA/1264, by SPP 1459 of DFG.

TT 93.4 Thu 10:15 H 0111

Investigation of atomic-scale strain variations in graphene as a function of applied strain — •Stefan E. Huber[1], Gerard Verbiest[2], Christoph Stampfer[2], and Karsten Reuter[1] — [1]Technische Universität München — [2]RWTH Aachen

Graphene exhibits unique electronic and mechanical properties. The very high electron mobilities that can be reached in state-of-the-art devices suggest this material to revolutionize present-day electronics. The demand for high mobilities raises the question what actually limits these in graphene. Recent experiments provide evidence that most likely nanometer-scale strain variations are the mechanism responsible for the limitation of the charge carrier mobility [1,2].

Homogeneously straining graphene is expected to reduce local strain fluctuations and thus to increase the electron mobility. We address this issue with atomistic simulations of two distinct mechanisms that may give rise to nanometer-scale strain variations in the presence of overall strain. Using (and comparing) a series of interatomic potentials to describe graphene, we study (i) the effect of surface defects in a hexagonal boron-nitride substrate deduced from first-principles DFT calculations as well as (ii) thermally induced fluctuations. In both respects, we discuss the effective suppression of out-of-plane distortions already at moderate global strains of a few per cent. In stark contrast, in-plane deformations are enhanced upon the application of global strain, a result clearly beyond the limitations of linear elasticity theory.

[1] N.J.G. Couto et al., Phys. Rev. X 4, 041019 (2014)
[2] S. Engels *et al.*, Phys. Rev. Lett. 113, 126801 (2014)

TT 93.5 Thu 10:30 H 0111

Uniformity of the pseudo-magnetic field in strained graphene — •Gerard Verbiest, Sascha Brinker, and Christoph Stampfer — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany

Graphene is a very promising candidate as active material in future electronic applications. However, its electrical properties are very sensitive to mechanical disturbances, as graphene is only one atomic layer thick. This coupling theoretically gives rise to a so-called "pseudo-vector field", and consequently to a "pseudo-magnetic field".

The pseudo-magnetic field can, just as a real magnetic field, induce Landau levels in graphene, if the field is strong enough. In order to utilize, i.e. measure this effect, one needs (i) a high sample quality and (ii) a large uniformity of the pseudo-magnetic field.

Here we present numerical simulations of the pseudo-magnetic field in graphene with a hexagonal shape as a function of tri-axial strain. We defined a radius of uniformity, as the radius for which the standard deviation from the pseudo-magnetic field in the center reaches 1%. For a hexagon with sides of 100 nm and a strain of 10%, the pseudo-magnetic field strength is ~40 T and is uniform within a diameter of 34 nm. For a hexagonal sample size with sides of 1 micron with a strain of 3.5%, the maximum pseudo-magnetic field is reduced to ~1.2 T, but it is uniform within a diameter of 540 nm.

TT 93.6 Thu 10:45 H 0111

Nanopores in Silicon Nitride Membranes, Graphene and CNM: Milling and Imaging Techniques at the Helium Ion Microscope — •Daniel Emmrich[1], Emanuel Marschewski[1], Achim Nadzeyka[2], Frank Nouvertné[2], Armin Gölzhäuser[1], and André Beyer[1] — [1]Physics of Supramolecular Systems, Bielefeld University, 33615 Bielefeld, Germany — [2]Raith GmbH, Konrad Adenauer Allee 8, 44263 Dortmund, Germany

The Helium Ion Microscope (HIM) is a charged particle microscope employing Helium ions for probing the sample. In the low dose regime, the HIM operates as microscope, high doses enable material modification and sputtering. Compared to conventional focussed ion beams (FIB) using metal ions like Gallium, the HIM offers a very small focal spot size down to 0.35 nm and a strongly localized sputter interaction with the material. We employ the HIM for both milling nanopores in free standing membranes as well as for the inspection of pores. The He+ beam with its unique properties overcomes the resolution limit of conventional FIB tools as we show in a comparison with a high resolution Ga-FIB. We achieve smallest He-milled nanopores with a diameter of about 4 nm in all investigated membranes: 30 nm thick Silicon Nitride, Graphene and 1 nm thick carbon nanomembranes (CNM) made from aromatic self-assembled monolayers by electron-induced cross-linking. Different strategies for the characterization of pores with the HIM will be discussed. In particular, we compare the feasibility of the ion generated secondary electron signal to the He+ transmission signal.

TT 93.7 Thu 11:00 H 0111

Doping of graphene on SiO_2 with N^+ and B^+ ions by low-energy ion irradiation. — •Steffen Weikert, Julian Alexan-

der Amani, and Hans Christian Hofsäss — II. Physikalisches Institut, Georg-August-Universität Göttingen, Deutschland

Its unique electrical properties make graphene a promising candidate for future electronic devices. An important milestone, especially for the industrial production of those devices, is the realization of a method for large-scale doping of graphene. A potential method for controlled doping of graphene, while minimizing the damage inflicted upon the sample, is low-energy ion irradiation.[1–3]
This work shows experiments on the irradiation of monolayer graphene on SiO_2 by N^+ and B^+ ions at 25 eV. For the experimental realization a mass-selected ion beam deposition system was used. [4] The irradiation was also simulated using the Monte Carlo program SDTrimSP. In addition to the irradiation of the graphene, I-V measurements were made before and after the irradiation.
[1] U. Bangert, W. Pierce, D. M. Kepaptsoglou, Q. Ramasse, R. Zan, M. H. Gass, J. A. Van den Berg, C. B. Boothroyd, J. Amani, and H. C. Hofsäss, Nano Lett. 2013, 13, 4902-4907.
[2] E. H. Åhlgren, J. Kotakoski, and A. V. Krasheninnikov, Phys. Rev. B (2011), 83, 115424.
[3] Y. Xu, K. Zhang, C. Brüsewitz, X. Wu, and H. C. Hofsäss, AIP Advances (2013), 3, 072120.
[4] H. Hofsäss, H. Binder, T. Klumpp and E. Recknagel, Diam. Relat. Mater. (1994), 3, 137.

15 min. break.

TT 93.8 Thu 11:30 H 0111

Field induced enhancement of refractive index and conductivity - a substrate effect in graphene — •Matthias Vaupel[1], Anke Dutschke[1], Ulrich Wurstbauer[2], and Frank Hitzel[3] — [1]Carl Zeiss Microscopy GmbH, Königsallee 9-21, 37081 Göttingen, Germany — [2]Dept. of Physics, Columbia University New York, NY 10027, USA — [3]DME Nanotechnologie GmbH, D-38106 Braunschweig, Germany

We study the effect of different substrates, conductive Si vs. isolating SiO2, on the electro-optic properties of graphene layers. To this end phase profiles of graphene layers were recorded by total interference contrast (TIC) microscopy, while atomic force microscopy measured the topography of the layers [1]. An optical model consistent with the measured height and phase profile of graphene yields the refractive index N and conductivity of graphene. Extraordinary high N = 3.9 + 9.2 i is obtained for the graphene on conductive substrate. The optical conductivity is 38 fold increased with respect to the reference value obtained on isolating substrate by TIC [1] and by ellipsometry [2]. These observations are mathematically consistent with the dielectric Drude function, which describes a damped harmonic electron oscillation with zero eigenfrequency and nonzero effective electron mass. The model applies for FETs and electro-optic devices made of graphene.

[1] M. Vaupel, A. Dutschke, U. Wurstbauer, F. Hitzel, A. Pasupathy, J.Appl.Phys. 114, (2013) 183107 [2] U. Wurstbauer, C. Röling, U. Wurstbauer, W. Wegscheider, M. Vaupel, P.H. Thiesen, D. Weiss, Appl. Phys. Lett. 97, (2010) 231901

TT 93.9 Thu 11:45 H 0111

Charge and spin transport in graphene nanoribbons with adatoms and defects — •Flaviano José Dos Santos[1,2], Filipe Souza Mendes Guimarães[1,2], and Roberto Bechara Muniz[1] — [1]Institute of Physics, Universidade Federal Fluminense, Niterói, Brazil — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Several features of spintronic systems are related to the spin-orbit coupling (SOC). Since SOC is relatively small in carbon atoms, several studies have been conducted in order to obtain a way to increase SOC in graphene (e.g., via adsorption of impurities on the graphene surface), which would allow to employ graphene as a basic material for spintronic devices. We have studied the charge and spin transport in graphene nanoribbons, in the linear response regime, affected by the presence of defects (vacancies and edge constrictions) and adatoms. We used effective models for light and heavy adsorbed impurities, some of them inducing enhancement of the SOC [1]. The results are obtained through a combination of analytical and numerical derivations. We investigated the impact of impurity concentration on the establishment of topologically protected edge states giving rise to a spin polarized current flux through the sample. In addition to conductance, local densities of states and current distribution calculations, we also simulate maps of real space local conductance properties for dual-probe Scanning Tunneling Microscope [2] setups on these systems. [1] C. Week *et al.*, Phys. Rev. X **1**, 021001 (2011). [2] M. Settnes *et al.*, Phys. Rev. Lett. **112**, 096801 (2014). Funding: Capes and CNPq (Brazil).

TT 93.10 Thu 12:00 H 0111

Electronic properties of Co atoms on Graphene / Ir(111) by photoelectron spectroscopy — •Michael Heber[1], Markus Scholz[1], Adrian Benz[1], Deniza Chekrygina[1], Michael Martins[1], and Wilfried Wurth[1,2] — [1]Physics Department and Center for Free-Electron Laser Science, Univ. Hamburg, 22761 Hamburg, Germany — [2]DESY Photon Science, 22607 Hamburg, Germany

Despite of the enormous achievements in our understanding of the interaction of deposited metal atoms with the underlying substrates, they still bear a variety of unexplored features. Recently, Graphene grown on metal substrates has proven to be a versatile template to create ordered arrays of adsorbed metal atoms. It was shown, that the electronic properties of adsorbed transition metal atoms strongly depend on the hybridization between the transition metal d-orbitals and the graphene π-band. The graphene π-band itself can hybridize with the valence states of the metal substrates. This opens a gateway to manipulate the adsorbate-Graphene interface itself and thus the electronic properties. We present core and valence level photoemission measurements of Co atoms deposited on Graphene/Ir(111) to obtain a detailed picture of the hybridization effects on the electronic structure of the metal atoms.This work is supported by the SFB 668 "Magnetism from single atoms to nanostructures"

TT 93.11 Thu 12:15 H 0111

hydration of bilayered graphene oxide — •bita rezania[1], nikolai severin[1], alexandr v talyzin[2], and jürgen p rabe[1] — [1]Humboldt University, Berlin, Germany — [2]Umeå University, Umeå, Sweden

Recently, it has been shown that graphene oxide (GO) membranes show remarkable selectivity in permeation of water molecules. This was attributed to the hydration of the membranes - the key to understand the water permeation mechanism. We investigated the change of the interlayer distance in bilayer GO as function of humidity and in liquid water using SFM [1]. The increase of relative humidity from 2 to *80% results in gradual expansion of interlayer distance by approximately 1 Å. The immersion into liquid water results in increase of the interlayer distance by another 3 Å. Our results are in good agreement with the averaged distance measured by X-ray diffraction on multilayered graphite oxides, which is commonly explained with an interstratification model. However, our experimental design excludes effects connected to interstratification. We find that the hydration is a continuous process of incorporation of water molecules into various sites within the GO layers, while liquid water inserts as a monolayer. The similarity of hydration for our bilayer and previously reported multilayered materials implies GO few and even bilayers to be suitable for selective water transport.

[1] Rezania, B., et al. Nano Lett. 2014, 14, 3993.

TT 93.12 Thu 12:30 H 0111

Humidity dependent oxygen transport through single layer graphene oxide — •Mohammad Fardin Gholami, Phillip Lange, Nikolai Severin, and Jürgen P. Rabe — Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

Graphene oxide (GO) is a strongly oxidized and nano-porous single sheet of graphene. Few layer thick GO membranes have been shown to exhibit molecular selective gas transport (H.W. Kim *et al.* and H. Li *et al.*, *Science*, 2013). The molecular selectivity is humidity dependent, which has been attributed to water molecules blocking either GO interlayers or pores. The latter would imply that also single layer GO may exhibit similar properties. Here we used the sensitivity of the fluorescence of thin films of a regioregular poly(3-hexylthiophene-2,5-diyl) to photo-oxidation in order to investigate the transport of oxygen through single layer GOs put on the polymer films by following its fluorescence decaying with time (P. Lange *et al.*, *J. Phys. Chem. C*, 2011). For samples exposed to humid mixtures of 80% nitrogen and 20% oxygen with 32% relative humidity we find that the fluorescence of the polymer covered by GO decays two times slower than the uncovered one. We did not observe any difference in the decay rates when the film was exposed to the corresponding dry gas mixture. We attribute the slower fluorescence decay of the polymer film covered by the humidified GO to slower permeation of oxygen molecules through GO pores clogged by the water molecules. This implies that even single layer GO can be

used as a humidity dependent molecular sieve.

TT 93.13 Thu 12:45 H 0111

In-situ Creation of Reduced Graphene Oxide Paper on Substrates — Peng Li[1], •Matthias M. L. Arras[2], Fuping Dong[2], Xin Wang[1,2], and Klaus D. Jandt[2] — [1]Department of Materials Science, Key Laboratory of Automobile Materials of MOE, Jilin University, Changchun, 130012, P. R. China — [2]Chair of Materials Science (CMS), Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Jena, Germany

Generally, the synthesis conditions of reduced graphene oxide paper (rGOP) require special substrates for its fabrication and, thus, it must often be transferred to application-suitable substrates, afterwards. Here, we tested the hypothesis that rGOP can be synthesized in-situ, e.g., on a polymer substrate, by using a mild step-by-step annealing of graphene oxide hydrosol. By applying the step-by-step annealing at 60, 100 and 160°C for 12 h, shiny and non-crimpling rGOP was created on polymer and glas substrates. The rGOP was characterized by Raman, infra red and X-ray photoelectron spectroscopy, as well as by optical and electron microscopy. Based on the results, a simple formation mechanism for the rGOP was proposed. The presented method will allow to equip surfaces with rGOP functionality directly and is also suitable for a patterned functionalization.

TT 94: Spin-Dependent Transport Phenomena I (organized by MA)

Time: Thursday 9:30–11:30 Location: H 0112

TT 94.1 Thu 9:30 H 0112

Unified theory for charge, spin and angular momentum excitations — •Filipe Souza Mendes Guimaraes[1,2], Antonio Tavares da Costa Jr[1], Roberto Bechara Muniz[1], Manuel dos Santos Dias[2], and Samir Lounis[2] — [1]Instituto de Física, Universidade Federal Fluminense, Niterói, Brazil — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The investigation of phenomena involving the spin and charge of the electron, called spintronics, has the potential to generate and enhance tools for the development of devices with low power consumption and fast switching speeds, as well as technologies that may be mass-produced. Polarized currents and angular momentum currents may be used to transfer information more efficiently than the conventional charge currents. We have developed a fully quantum mechanical approach that allows us to study charge, spin and angular momentum excitations. This method takes into account realistic electronic structures obtained from first principles calculations. We show that spin, charge and angular momentum currents and disturbances can be expressed in terms of generalized susceptibilities. Results on static and dynamic quantities related to the Spin Hall Effect and Inverse Spin Hall Effect for ultrathin films of Pt and Co/Pt will be presented.

TT 94.2 Thu 9:45 H 0112

Enhancement of the anomalous Hall effect in ternary alloys — •Katarina Tauber[1], Albert Hönemann[1], Dmitry Fedorov[2,1], Martin Gradhand[3], and Ingrid Mertig[1,2] — [1]Martin Luther University Halle-Wittenberg — [2]Max Planck Institute of Microstructure Physics, Halle — [3]University of Bristol

We present our results for the anomalous Hall effect (AHE) in ternary alloys of the form $Cu(Mn_{1-w}T_w)$ with T as nonmagnetic Au, Bi, Ir, Lu, Sb, or Ta impurities. As was shown experimentally [1], Mn causes negligible skew scattering in copper and therefore a very weak AHE is observed in the Cu(Mn) binary alloys. In contrast, the systems Cu(T) have a strong skew scattering, but only provide a spin Hall effect (SHE) instead of an AHE, since the systems are nonmagnetic. Fert *et al.* [1] found that the AHE can be strongly enhanced in the Cu(Mn) alloys via the co-doping of 5*d*-impurities. Furthermore, they showed that it is possible to describe the SHE in the Cu(T) alloy via measurements of the AHE in the $Cu(Mn_{1-w}T_w)$ alloys. Here, a theoretical study via Matthiessen's rule is presented with focus on the connection between the AHE in the ternary alloy and the SHE in the related Cu(T) alloy. Our formalism provides the conditions for a maximal enhancement of the AHE with respect to the weighting factor w. This is underpinned by first-principles calculations using a relativistic Korringa-Kohn-Rostoker method and Boltzmann transport theory [2].

[1] A. Fert et al., JMMM **24**, 231 (1981).

[2] K. Tauber et al., Phys. Rev. B **87**, 161114(R) (2013).

TT 94.3 Thu 10:00 H 0112

Anomalous Hall Effect at Terahertz Frequencies — Tom Seifert[1], Frank Freimuth[2], Lukas Braun[1], Florin Radu[3], Ulrike Martens[4], Markus Münzenberg[4], Ilie Radu[3], Yuriy Mokrousov[2], Martin Wolf[1], and •Tobias Kampfrath[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Forschungszentrum Jülich, Peter Grünberg Institut, 52425 Jülich, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [4]Ernst-Moritz-Arndt Universität, Institut für Physik, Felix-Hausdorff-Str. 6, 17489 Greifswald, Germany

Spin-orbit interaction (SOI) is expected to be of central importance in future spin-based electronics (spintronics) as it permits, for example, the conversion of charge into spin currents. It is highly interesting to study SOI-based effects at terahertz (THz) frequencies because (i) spintronic devices should eventually operate at THz rates and since (ii) the THz photon energy (4 meV at 1 THz) is comparable to the SOI energy in magnetically ordered solids. Here, we employ broadband THz time-domain ellipsometry [1] to measure the complex conductivity tensor of various magnetic metals from 1 to 40 THz. Supported by *ab initio* calculations [2], we discuss spectral features of the spin Hall angle in terms of SOI.

[1] A. Rubano, L. Braun, M. Wolf, and T. Kampfrath, Appl. Phys. Lett. **101**, 081103 (2012).

[2] F. Freimuth, S. Blügel, and Y. Mokrousov, Phys. Rev. Lett. **105**, 246602 (2010).

TT 94.4 Thu 10:15 H 0112

Separation of different contributions to the spin Hall effect in dilute alloys based on the Kubo-Středa approach — •Kristina Chadova[1], Dmitry Fedorov[2,3], Christian Herschbach[2], Martin Gradhand[4], Ingrid Mertig[2,3], Diemo Ködderitzsch[1], and Hubert Ebert[1] — [1]Department of Chemistry, Physical Chemistry, Ludwig-Maximilians University Munich, Germany — [2]Institute of Physics, Martin-Luther University Halle-Weinberg, 06099 Halle, Germany — [3]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany — [4]H.H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, United Kingdom

In recent years several first-principles approaches have been established to describe transverse electron transport phenomena as e.g. the anomalous Hall and spin Hall effects. Starting from an earlier decomposition scheme [1] we extract the coherent part of the SHC as well as the extrinsic vertex-correction (vc) based skew-scattering and the side jump (sj) contributions. Further using insight from Boltzmann transport theory we separate the sj into a sum of a term being exclusively caused by the vc and a term that does not depend on the vc. The proposed procedure was applied within first-principles fully relativistic KKR transport framework (Kubo-Středa) to dilute alloys based on Cu, Au and Pt hosts [2].

[1] S Lowitzer, D Ködderitzsch, H Ebert, PRL **105**, 266604 (2010)

[2] K Chadova, D Fedorov, C Herschbach, M Gradhand, I Mertig, D Ködderitzsch, H Ebert (to be published)

TT 94.5 Thu 10:30 H 0112

Higher dimensional Wannier functions for a description of multi-parameter ab initio Hamiltonians — •Jan-Philipp Hanke, Frank Freimuth, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Maximally localized Wannier functions (MLWFs) have become a widely applied tool in understanding the electronic structure [1]. Here, we present higher dimensional Wannier functions (HDWFs), which provide a minimal and accurate description of multi-parameter Hamiltonians $H^{(\mathbf{k},\boldsymbol{\lambda})}$ carrying a dependence on the crystal momentum $\mathbf{k}$ and an additional periodic parameter $\boldsymbol{\lambda}$. We derive a generalized interpolation scheme and emphasize the essential conceptual and computational

simplifications in using the formalism for instance in the evaluation of linear response coefficients. The necessary machinery to construct HD-WFs from *ab initio* is implemented within the full-potential linearized augmented plane-wave method (FLAPW) as realized in the FLEUR code [2]. We further apply our implementation to accurately interpolate the Hamiltonian of a one-dimensional magnetic chain of Mn atoms with spin-spiral texture in a composite space of Bloch and spin-spiral vectors, and thereby extract efficiently Heisenberg exchange constants.

Financial support by the HGF-YIG programme VH-NG-513 and SPP 1538 of DFG is gratefully acknowledged.

[1] N. Marzari and D. Vanderbilt, Phys. Rev. B **65**, 12847 (1997).
[2] See http://www.flapw.de

TT 94.6 Thu 10:45 H 0112

Description of electron transport in multilayer systems using Boltzmann approach — •Ondřej Stejskal[1], André Thiaville[2], Shunsuke Fukami[3], Hideo Ohno[3], and Jaroslav Hamrle[1] — [1]IF, VSB-Technical University of Ostrava, Czech Republic — [2]LPS, Univ. Paris-Sud, Orsay, France — [3]CSIS/RIEC/WPI-AIMR, Tohoku University, Sendai, Japan

Recent discoveries of spin current, spin Hall effect and Rashba effect have attracted a new interest in transport phenomena in multilayer systems. The Fuchs-Sondheimer theory that is based on the Boltzmann transport equation covers the transport phenomena in thin films. Though the paper was released in 1952, the theory is still being used with great success and is in a great agreement with experiments. We use this theory for the description of an in-plane current density in a multilayer system Ta/Pt/[Co/Ni]/Pt/Ta. The resistance of the multilayer is measured as the function of the thicknesses of individual layers. Using the Fuchs-Sondheimer model, we obtain the material and interface parameters of the layers and the current distribution in the sample. This is of a great importance for multilayers, as the spin phenomena, like spin Hall effect and spin-transfer torque, are proportional to current densities in the vicinity of the interface with ferromagnetic material. This work is partly supported by R&D Project for ICT Key Technology to Realize Future Society of MEXT.

[1] E. Sondheimer, Advances in Physics 1, 1 (1952)
[2] P. M. Haney, H.-W. Lee, K.-J. Lee, A. Manchon, M. D. Stiles, Physical Review B., 87, 174411 (2013)

TT 94.7 Thu 11:00 H 0112

Higher order contributions to Anisotropic Interface Magnetoresistance (AIMR) in Ni/Pt thin films — •Afsaneh Farhadi, André Kobs, Gerrit Winkler, Carsten Thönnissen, and Hans Peter Oepen — Institut für Nanostruktur- und Festkörperphysik, Universität Hamburg, Jungiusstr. 11a, 20355 Hamburg, Germany

The influence of interfaces on the magnetotransport in systems with one ferromagnetic layer has attracted much attention. In Pt/Co/Pt the resistivity behaves as $\rho(\varphi,\theta) = \rho_t + \Delta\rho_{ip}\cos^2\varphi\sin^2\theta + \Delta\rho_{op}\cos^2\theta$ where φ/θ is the angle between magnetization and current direction/film normal [1]. While $\Delta\rho_{ip}$ is caused by the conventional AMR (bulk effect) a $\Delta\rho_{op} \propto 1/t$ behavior was found for Pt(5nm)/Co(t)/Pt(3nm) sandwiches revealing that $\Delta\rho_{op}$ originates at the Co/Pt interfaces (anisotropic interface magnetoresistance (AIMR)). So far the AIMR was observed also for Py/Pt and Co/Pd [2,3]. In order to answer the question if interfacial MR contributions also exist when stacking isoelectronic materials we investigated Ni/Pt systems. We prepared Pt(5nm)/Ni(t)/Pt(3nm) sandwiches with Ni thicknesses of $1-50$ nm by dc magnetron sputtering on Si_3N_4 substrate. As a result, in contrast to previous findings, the $\rho(\theta)$ behavior can only be satisfactorily described when considering higher orders in the expansion of the MR up to $n=3$: $\rho(\theta) = \rho_t + \sum_n \Delta\rho_{op,2n}\cos^{2n}\theta$. The thickness dependence of the amplitudes $\Delta\rho_{op,2n}$ behaves according to $1/t$ revealing that also the higher orders have their origin at the Ni/Pt interfaces.

[1] A. Kobs et al., PRB **90**, 016401 (2014), [2] Y.M. Lu et al., PRB **87**, 220409 (2013), [3] J.-C. Lee et al., JAP **113**, 17C714 (2013).

TT 94.8 Thu 11:15 H 0112

Lattice strain accompanying the colossal magnetoresistance effect in EuB_6 — •Rudra Sekhar Manna[1,2], Pintu Das[1], Mariano de Souza[1], Frank Schnelle[1], Michael Lang[1], Stephan von Molnár[3], Zachary Fisk[4], and Jens Müller[1] — [1]Phys. Inst., Goethe-University Frankfurt, 60438 Frankfurt (Main), SFB/TR49, Germany — [2]EP VI, EKM, Augsburg University, 86159 Augsburg, Germany — [3]Phys. Dept., FSU, Tallahassee, Florida 32306, USA — [4]Phys. Dept., UC Irvine, California 92697, USA

Semimetallic EuB_6 shows a complex ferromagnetic order and a colossal magnetoresistance effect due to the interplay of magnetic, electronic and lattice degrees of freedom. EuB_6 may be viewed as a model system, where pure magnetism-tuned transport and the response of the crystal lattice can be studied in a comparatively simple environment, i.e., not influenced by strong crystal-electric field effects and Jahn-Teller distortions. We performed thermal expansion and magnetostriction measurements and find a large lattice response when the system enters the ferromagnetic region. Our analysis reveals that a significant part of these lattice effects - quantified by the large magnetic Grüneisen parameter and spontaneous strain when entering the ferromagnetic region - originates in the magnetically driven delocalization of charge carriers, consistent with the scenario of percolating magnetic polarons. A strong effect of the formation and dynamics of local magnetic clusters on the lattice parameters is suggested to be a general feature of colossal magnetoresistance materials [1].

[1] R. S. Manna *et al.*, PRL **113**, 067202 (2014)

TT 95: Spintronics: Mobile Electrons and Holes (jointly with HL, MA)

Time: Thursday 10:00–12:30 Location: ER 164

TT 95.1 Thu 10:00 ER 164

Conserved Spin Quantity in Strained Hole Systems with Rashba and Dresselhaus Spin-Orbit Coupling — •Michael Kammermeier[1], Paul Wenk[1], John Schliemann[1], Klaus Richter[1], and Roland Winkler[2] — [1]Universität Regensburg, D-93040 Regensburg, Germany — [2]Northern Illinois University, IL 60115 DeKalb, US

We investigate conditions for the existence of a conserved spin quantity in two-dimensional hole gases in zincblende type semiconductor heterostructures. It is shown that in the presence of shear stress, a symmetric in-plane strain, and both Rashba and Dresselhaus spin-orbit coupling one can find such a conserved quantity. The found optimal parameter-space, for strain and spin-orbit coupling strength, gives the possibility to an experimental access. This is in contrast to previous works which require restrictions on the band model parameters (here the Luttinger parameters) which are either difficult to realize in real materials or even singular ($\gamma_3 = 0$).

* * *

[1] Schliemann *et al.*, PRL **90** 146801 (2003)
[2] Bernevig *et al.*, PRL **97** 236601 (2006)
[3] Kohda *et al.*, PRB **86** 081306 (2012)
[4] Dollinger *et al.* Phys. Rev. B **90**, 115306 (2014)

TT 95.2 Thu 10:15 ER 164

Quantum transport and response with spin-orbit coupling in magnetic fields — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Electronic transport in spin-polarized systems with impurity interactions and spin-dependent meanfields is discussed. The coupled quantum kinetic equations for the scalar and spin components for SU(2) are derived with special consideration of spin-orbit coupling and magnetic fields. Linearizing, the RPA spin and density dynamical responses to electric fields (polarized light) are preseented for arbitrary magnetic fields, Several known effects are described: spin-Hall, anomalous Hall and optical Hall effect, spin-heat coupling. New transport coefficients occur due to the selfconsistent precession direction. Clarifying the relative importance of meanfield and scattering correlations, new modes due to magnetic fields and spin-orbit coupling are found. (EPL, 104 (2013) 2700)

TT 95.3 Thu 10:30 ER 164

Spin injection through Fe/GaAs Schottky contacts —

•Lennart-Knud Liefeith, Rajkiran Tholapi, Max Hänze, Ann-Kathrin Michel, Taras Slobodskyy, and Wolfgang Hansen — Institut für Festkörper- und Nanostrukturphysik, Hamburg, Hamburg

The understanding of the dominant mechanism of spin injection through the Fe/GaAs interface is crucial for spintronics applications. It was suggested that the spin injection process is controlled by thermal activation of surface states at the ferromagnet/semiconductor interface [1]. To test this theory we investigated the bias dependence of the spin injection efficiency as well as the electrical properties of the interface. The measurements were carried out using non-local spin detection devices at liquid helium temperatures and backed up by magneto optical Kerr effect and magnetic force microscopy measurements on the electrodes. We found that the post growth annealing strongly influences the spin injection efficiency and a notable asymmetry of the spin injection efficiency depending on the applied bias was observed.

[1] Q. U. Hu et. al., „Spin accumulation near Fe/GaAs(001) interfaces: The role of semiconductor band structure“, Physical Review B 84, 085306 (2011)

TT 95.4 Thu 10:45 ER 164

Electric control of spin transport in GaAs (111)B quantum wells — •Alberto Hernández-Mínguez, Klaus Biermann, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The main challenge towards the use of electron spins in semiconductors is the control of the dephasing mechanisms that reduce the spin lifetime below the spin manipulation time. In III-V semiconductors, the main relaxation processes are related to the spin-orbit interaction (SOI). In the case of GaAs(111) quantum wells (QWs), the SOI can be efficiently suppressed for out-of-plane spins by applying an electric field, E_z, transverse to the QW plane. In this case, the contribution to the SOI induced by E_z compensates the intrinsic SOI due to the zinc-blende lattice and spin lifetimes of tenths of ns are observed.

In this contribution, we show experimental studies of both carrier and spin diffusion in a GaAs(111) QW under the effect of vertical electric fields. Spin polarized electron-hole pairs are optically generated in the QW by a tightly focused laser beam. The carrier and spin dynamics are studied by spatially and time-resolved photoluminescence. We show that the enhancement of the spin lifetime due to SOI compensation allows the transport of out-of-plane electron spins over distances exceeding 10 μm. In addition to the spin lifetime, the spin diffusion coefficient D_s also depends on E_z. For the carrier densities and temperatures studied, D_s shows a maximum of approx. 50 cm^2/s at SOI compensation, where it approaches the values observed for the carrier diffusion coefficient under the same experimental conditions.

TT 95.5 Thu 11:00 ER 164

Time and space resolved visualization of spin diffusion and drift in GaAs based two-dimensional electron gases — •Markus Schwemmer[1], Roland Völkl[1], Tobias Korn[1], Sergey Tarasenko[2], Dieter Schuh[1], Dominique Bougeard[1], Mariusz Ciorga[1], Werner Wegscheider[3], and Christian Schüller[1] — [1]Institute of Experimental and Applied Physics, Faculty of Physics, University of Regensburg, Germany — [2]A. F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, St. Petersburg, Russia — [3]ETH Zurich, Switzerland

The combination of a femtosecond pulsed TiSa-Laser system with a magneto-optical Kerr effect microscope setup allows us to study time and space resolved propagation of an optically injected electron spin packet in a resident two-dimensional electron gas based on a modulation-doped AlGaAs/GaAs quantum well. The interplay between the Dresselhaus and Rashba fields according to crystallographic orientation and layer structure of the sample determines the electron spin dynamics. On one hand we present diffusive and current-driven motion of a spin packet in a sample in which the orientation of the optically injected spins point along the effective spin orbit field. Therefore D'yakonov-Perel spin dephasing is suppresed and a long spin coherence time can be attained. On the other hand the diffusive spreading of the initial spin packet in a sample with a spin-orbit interaction close to the spin helix regime is monitored, whereby a direct visualization of the helix pattern is achieved. Financial support by the DFG via SFB 689 and SPP 1285 is gratefully acknowledged.

Coffee break

TT 95.6 Thu 11:30 ER 164

Hole spin coherence in coupled GaAs/AlAs quantum wells — •Christian Gradl, Johannes Holler, Michael Kempf, Dieter Schuh, Dominique Bougeard, Christian Schüller, and Tobias Korn — Universität Regensburg, D-93040 Regensburg, Germany

We performed time-resolved Kerr rotation (TRKR) measurements on an undoped [113]-grown double quantum well (QW) structure to resolve the spin dynamics of hole ensembles at low temperatures. Our gated system consists of two QWs with different well widths, which we use for the spatial separation of the optically excited electron-hole pairs. Thus, we are able to create hole ensembles with spin dephasing times of several hundreds of picoseconds in the broader QW without any doping.

This allowed an unexpected observation of a non-precessing component in the TRKR signal in the presence of an applied magnetic field perpendicular to the spin polarization. These measurements also show the non-precessing component to be a part of the optically generated hole spin polarization. This effect might arise from a tilting of the quantization axis with respect to the applied magnetic field due to a large anisotropy between the in- and out-of-plane hole g factor.

TT 95.7 Thu 11:45 ER 164

Inelastic light scattering in a two-dimensional electron gas under external magnetic fields — •Christoph Schönhuber, Dieter Schuh, Dominique Bougeard, Tobias Korn, and Christian Schüller — Universität Regensburg, 93040 Regensburg, Germany

We present inelastic light scattering measurements of a 12-nm-wide (001)-oriented GaAs/AlGaAs QW under external magnetic fields. The investigated system is single-side Si doped to reach a balanced Rashba and Dresselhaus SOI contribution.

The performed measurements on intrasubband transitions of the conduction band reveal for B=0 a double peak structure for the [1-1] direction due to spin splitting, while the [11] direction features only a single peak. For small magnetic fields, the wave vector appears to be conserved in the scattering process while both directions aim to assimilate the excitation with increasing field strength. At higher perpendicular magnetic fields, the anisotropic behaviour has vanished and the spectra are characterized by inter-Landau excitations.

TT 95.8 Thu 12:00 ER 164

Impurity band spin dynamics in GaAs directly above the metal-to-insulator transition — •Jan Gerrit Lonnemann[1], Eddy Patrick Rugeramigabo[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Institute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Laboratory of Nano and Quantum Engineering, Leibniz Universität Hannover, Schneiderberg 39, D-30167 Hannover, Germany

Several theoretical works treat the spin dynamics in zinc-blende semiconductors. We present extremely low excitation Hanle depolarization measurements on well characterized n-doped MBE grown GaAs in the vicinity of the metal-to-insulator transition (MIT). The doping concentrations range from the MIT at $2 * 10^{16}$ cm^{-3}, where extremely long spin lifetimes are experimentally observed [1], up to the merging of impurity and conduction band at $8 * 10^{16}$ cm^{-3}, where for conduction band electrons the spin relaxation is typically dominated by the Dyakonov-Perel mechanism (DP). We conclude from our measurements that DP is also dominating the impurity band regime in slightly metallic samples. Furthermore the measurements show no indication of spin relaxation by hopping transport (HT) that has recently been predicted as the main mechanism of relaxation for the impurity band regime [2]. In contrast our measurements of the spin dynamics indicate a metal-like behavior of the electrons in the impurity band.

[1] M. Römer et al.; *Phys. Rev. B*, **81**, 075216 (2010).
[2] G.A. Intronati et al.; *Phys. Rev. Lett.*, **108**, 016601 (2012).

TT 95.9 Thu 12:15 ER 164

Boundary dependent spin manipulation via Rashba-SOC — •Phillipp Reck and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Besides spin injection, controlled spin manipulation is a major aspect of active spintronic devices such as spin transistors. In a two dimensional electron gas (2DEG), this manipulation is often achieved by Rashba spin orbit coupling (SOC).

We study numerically the effects of a non-trivial deformation of a wire (quasi 1DEG) on the spin evolution of an initially spin polarized wave packet exposed to Rashba SOC. To make sure that the wave packet follows the deformation, we apply additionally a magnetic field

to get edge states, which are resistant to impurity scattering. The benefit of the deformation is the higher variability of the spin state: Without the deformation, the spin precesses on the Bloch sphere around one fixed axis, whereas the deformation changes continuously the orientation of the precession axis leading to a more complex spin evolution. Thus, it is possible, e. g., to create either a x-, y- or z-spin polarization by only changing the Rashba SOC, but not the geometry.

A generalization is a wire with a periodic deformation. Because of the constant out-of-plane magnetic field and an in-plane rotating effective magnetic field due to SOC, one could engineer spin resonance effects.

TT 96: Frontiers of Electronic Structure Theory: 2D TMDC and Excitonic Effects (organized by O)

Time: Thursday 10:30–13:15 Location: MA 004

Invited Talk TT 96.1 Thu 10:30 MA 004

Interaction and Correlation Effects in Quasi Two-dimensional Materials — •Steven G. Louie — Physics Department, University of California at Berkeley, and Lawrence Berkeley National Lab, Berkeley, CA 94720 USA

Experimental and theoretical studies of atomically thin quasi two-dimensional materials and their nanostructures have revealed that these systems can exhibit highly unusual behaviors. Owing to their reduced dimensionality, these systems present opportunities for manifestation of concepts/phenomena that may not be so prominent or have not been seen in bulk materials. Symmetry and many-body interaction effects often play a critical role in shaping qualitatively and quantitatively their properties. In this talk, we present some theoretical studies on graphene as well as other quasi-2D systems such as monolayer and few-layer transition metal dichalcogenides (e.g., MoS2, MoSe2, WS2, and WSe2) and metal monochalcogenides (such as GaSe and FeSe). Several quantum phenomena are discussed, including novel and dominant exciton effects, tunable magnetism, electron supercollimation by disorder, unusual plasmon behaviors, and possible enhanced superconductivity in some of these systems. We investigate their physical origins and compare theoretical predictions with experimental data.

TT 96.2 Thu 11:00 MA 004

Screening of the Coulomb interaction in two-dimensional semiconductors: The case of transition metal dichalcogenides — •Ersoy Sasioglu, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute forAdvanced Simulation, Forschungszentrum Jülich and JARA, 52425Jülich, Germany

Experimentally determined large exciton binding energies and nonhydrogenic Rydberg series in monolayer transition metal (TM) dichalcogenides indicate a long-range behavior of the Coulomb interaction. By means of first-principles calculations in conjunction with the random-phase approximation [1,2] within the FLAPW method [3] we study screening of the Coulomb interaction in two-dimensional semiconducting TM dichalcogenides MX_2 (M=Cr, Mo, W; X=S, Se). We show that the screening in these systems deviates substantially from the bulk behavior, i.e., the short-range interaction is strongly screened, while the long-range interaction is anti-screened. This unconventional screening reduces the gradient of the Coulomb interaction giving rise to weak correlation effects, which explains the experimentally observed large exciton binding energies as well as the success of the one-particle density functional theory in the description of the electronic structure of these systems. This work has been supported in part by DFG-FOR-1346.

[1] C. Friedrich *et al.*, Phys. Rev. B. **81**, 125102 (2010).
[2] E. Şaşıoğlu *et al.*, Phys. Rev. B **83**, 121101(R) (2011).
[3] www.flapw.de

TT 96.3 Thu 11:15 MA 004

Ultra-fast transient absorption spectra of monolayer MoS2 by first principle — •Margherita Marsili[1], Deborah Prezzi[1], Davide Sangalli[2], and Andrea Marini[2] — [1]CNR Istituto di Nanoscienze S3, Modena, Italy — [2]CNR ISM, Montelibretti, Italy

We compute ultrafast transient absorption spectra of MoS2 monolayers by employing a novel approach which combines density-functional and non-equilibrium Green's function theories. This approach allows the description of pump-probe optical experiments where the system is excited by an ultrashort laser pulse, and the variation of the optical response is probed at different time delays, thus providing a wealth of information on the fundamental physics of the relaxation processes. The case of monolayer MoS2 is extremely challenging due to the interplay of excitonic, electron-phonon and spin-orbit coupling effects. We describe the excitation of the MoS2 electronic system and follow the subsequent dynamics using a fully non-collinear spin formulation of the theory, including excitonic effects. The results are compared with experimental pump-probe data.

TT 96.4 Thu 11:30 MA 004

Plasmon and exciton dispersion in two dimensions — •Pier Luigi Cudazzo — LSI Ecole Polytechnique and ETSF, Palaiseau, France

Understanding the electronic properties of 2D materials requires the investigation of their elementary excitations that dictate their optical and transport properties. Using state-of-the-art Green's function many body approach we present a first principle study of the collective excitations (namely excitons and plasmons) in 2D materials. In particular from the evaluation of the dielectric function we investigated the exciton dispersion in graphane and hBN and the plasmon dispersion in metallic TMDs[1-3]. From our results we provide an exact analytic form of the two-dimensional screened potential. In contrast to 3D systems where the macroscopic screening can be described by a static dielectric constant in 2D systems the macroscopic screening is non local (q-dependent) showing a logarithmic divergence for small distances and reaching the unscreened Coulomb potential for large distances[4].

[1] P. Cudazzo, et. al. New J. Phys. 15 125005 (2013). [2] P. Cudazzo, et. al. (in preparation) [3] P. Cudazzo, et. al. Phys. Rev. Lett. 104 226804 (2010). [4] P. Cudazzo, et. al. Phys. Rev. B 84 085406 (2011).

TT 96.5 Thu 11:45 MA 004

Origin of metallic edge states in transition-metal-dichalcogenide nanostructures — •Marco Gibertini and Nicola Marzari — Theory and Simulation of Materials (THEOS) and National Center for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Switzerland

The existence of metallic edge states in transition-metal-dichalcogenide nanostructures has been reported both in the experimental and theoretical literature. Such nanostructures include for instance triangular islands and zigzag nanoribbons. Nonetheless, a thorough understanding of the mechanism giving rise to metallic states at the edge of such bulk insulating materials is still missing. Here we suggest a possible origin of such states and support our findings with first-principles density-functional-theory simulations. The key observation is that transition metal dichalcogenides like MoS_2 display a finite *formal* polarization that induces a charge reconstruction with the appearance of free carriers at the edges. We also suggest possible innovative applications in nanoelectronics and solar-energy devices.

TT 96.6 Thu 12:00 MA 004

Starting-point dependence in the Bethe-Salpeter equation: example of rutile TiO_2 — •Olga Turkina, Ute Werner, Dmitrii Nabok, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Zum Großen Windkanal 6, D-12489 Berlin, Germany

Many-body perturbation theory, combining the GW approach and the Bethe-Salpeter equation (BSE), is a powerful tool for the description of one- and two-particle excitations. However, employing density functional theory as a starting point for these methods may lead to results that depend on the choice of the exchange-correlation (xc) functional. This starting-point dependence is well known for the G_0W_0 approximation. Such dependence is expected to occur also for BSE calculations, however, has not yet been investigated. With the example of

rutile TiO_2, we show that this is, indeed, the case. We employ two different xc functionals: the generalized gradient approximation (PBE) and a hybrid functional (PBE0'), combining a fraction of 25% exact exchange with PBE. The electronic structure is calculated using the G_0W_0 approximation. The BSE is solved to obtain the optical absorption spectra. These are analyzed with regard to the influence of eigenvalues, wave functions, and screening as originating from different xc functionals.

TT 96.7 Thu 12:15 MA 004

Efficient exchange-correlation kernels for the description of excitonic effects in solids — •Santiago Rigamonti[1,4], Silvana Botti[2,4], Valérie Veniard[3,4], Claudia Draxl[1,4], Lucia Reining[3,4], and Francesco Sottile[3,4] — [1]Physics Department, Humboldt-Universität zu Berlin, Germany — [2]Friedrich-Schiller Universität Jena, Institut für Festkörpertheorie und -optik — [3]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, F-91128 Palaiseau, France — [4]European Theoretical Spectroscopy Facility (ETSF)

One of the major challenges for time-dependent density-functional theory is the accurate and efficient description of excitonic effects in solids, captured by the exchange-correlation (xc) kernel. In a recent empirical approach, the so-called "bootstrap" kernel has been proposed. Due to its high efficiency and some promising results [1] it appeared indeed interesting. In this work, we find a physically motivated derivation for it, opening the way to understand its weaknesses and to propose a new xc kernel. Our kernel is both simpler and more reliable, as confirmed by our numerical results [2]. We also propose a simple method to estimate exciton binding energies from the dielectric functions computed in the random-phase approximation alone. This method makes the approach accessible to a wide range of scientists.

[1] S. Sharma, J. K. Dewhurst, A. Sanna, and E. K. U. Gross, *Phys. Rev. Lett.* **107**, 186401 (2011).
[2] S. Rigamonti, S. Botti, V. Veniard, C. Draxl, L. Reining, and F. Sottile, *submitted*.

TT 96.8 Thu 12:30 MA 004

Excitonic effects in many-body calculations — •Matteo Gatti[1,2], Igor Reshetnyak[1], Giorgia Fugallo[1], Pierluigi Cudazzo[1], Francesco Sottile[1], and Lucia Reining[1] — [1]LSI, CNRS-Ecole Polytechnique and ETSF, Palaiseau, France — [2]Synchrotron Soleil, Gif-sur-Yvette, France

The Bethe-Salpeter equation (BSE) is the state-of-art approach to calculate the absorption spectra of a large variety of materials [1]. Here we show that that the BSE is a powerful and accurate method also for the calculation of the exciton dispersion [2-4] (i.e. the exciton energy as a function of the momentum q carried by the electron-hole pair), and of the off-diagonal elements of the dielectric function in reciprocal space $\epsilon_{G,G'}(q,\omega)$ [5]. On the one hand, this allows the ab initio simulation of spectra measured by Electron Energy-Loss Spectroscopy (EELS) and Inelastic X-ray Scattering (IXS), including its Coherent version (CIXS), well beyond the optical limit $q \to 0$. On the other hand, this opens the door to the calculation of spectral functions [6-8] using the cumulant expansion for the Green's function G with a screened Coulomb interaction W that includes excitonic effects beyond the random-phase approximation employed in the GW approximation.

[1] G. Onida, *et al.*, Rev. Mod. Phys. **74**, 601 (2002). [2] M. Gatti and F. Sottile, Phys. Rev. B **88**, 155113 (2013). [3] P. Cudazzo, *et al.*, Phys. Rev. B **88**, 195152 (2013). [4] G. Fugallo, *et al.*, unpublished. [5] I. Reshetnyak, *et al.*, unpublished. [6] M. Guzzo, *et al.*, Phys. Rev. Lett. **107**, 166401 (2011). [7] M. Gatti and M. Guzzo, Phys. Rev. B **87**, 155147 (2013). [8] M. Guzzo, *et al.*, Phys. Rev. B **89**, 085425 (2014).

TT 96.9 Thu 12:45 MA 004

Efficient parameter-free calculation of absorption spectra for insulators, semiconductors and metals from time-dependent current DFT — •Arjan Berger — LCPQ - IRSAMC, Université de Toulouse III - Paul Sabatier, CNRS, Toulouse, France and European Theoretical Spectroscopy Facility

In this work we show that with a simple dynamical kernel we can obtain good absorption spectra from time-dependent current-density functional theory (TDCDFT) for insulators, semiconductors and metals. Our approach is fully parameter free since no artificial broadening parameter is used to match calculated and measured spectra. The cost of a calculation is equal to an RPA calculation. Moreover, our TDCDFT approach scales better with system size than standard TDDFT implementations.

TT 96.10 Thu 13:00 MA 004

Optical excitations in MoS_2 within ab-initio many-body perturbation theory — •Matthias Drüppel, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

The transition metal dichalcogenides (TMDC), and MoS_2 as its most prominent member, open the door to a field of two dimensional atomically thin semiconductors which offer rich physics.

The state of the art theoretical description of electronic excitations in these materials starts with density-functional calculations (DFT), followed by the GW method in combination with a solution of the Bethe-Salpeter equation. The *converged* calculation (especially with respect to the size of the basis, i.e. number of plane waves, and k-meshs) of the last two steps has shown to be numerically extremely challenging.

We apply the efficient LDA+GdW [1] approach to the excited states which enables us to describe electronic excitations in MoS_2 at substantially lower numerical cost. In the LDA+GdW approximation the quasiparticle self-energy corrections to the LDA-DFT energies result from the difference between the correct screening (semiconducting) and hypothetical metallic screening.

This approach sets us in a position where more atoms per unit cells can be treated, e.g., for defects and for MoS_2 on substrates.

[1] M. Rohlfing, Phys. Rev. B. **82**, 205127 (2010)

TT 97: Graphene: Structure (jointly with O, HL)

Time: Thursday 10:30–13:00 Location: MA 041

TT 97.1 Thu 10:30 MA 041

Manganese Intercalation in Graphene/Ir(111): a structural study — •Stefan Böttcher[1], Hendrik Vita[1], Yuriy S. Dedkov[2], and Karsten Horn[1] — [1]Fritz-Haber Institute, Faradayweg 4-6, 14195 Berlin — [2]SPECS Surface Nano Analysis GmbH, Voltastrasse 5, 13355 Berlin

The graphene/substrate interaction is of interest for a many applications, and to understand and classify the interaction mechanism as such. For example, the 3d transition metals Fe, Co and Ni on the one hand, and Cu on the other suggest that a classification into strongly and weakly interacting systems may be possible, as judged by criteria such as the survival of the Dirac cone or the crystallographic structure of the graphene layer. Here we present a structural study, through LEED and STM, of manganese intercalation on graphene/Ir(111), a system that has so far not been studied. We follow the stages of the intercalation process, from the deposition of Mn on top through the formation of the intercalated phase. Manganese is found to be arranged pseudomorphically to the Ir(111) substrate underneath graphene. While several criteria for a weak interaction are fulfilled, the graphene/Mn/Ir(111) system also shows structural evidence for a strong interaction between the graphene and the Mn layer, e.g. a lower separation between graphene and the intercalated layer, a conclusion that is further supported by ARPES. Manganese intercalation may therefore be special because it fills the gap between the strongly and weakly interacting transition metals. In addition, at higher intercalation temperatures a new, possibly surface alloyed phase is observed.

TT 97.2 Thu 10:45 MA 041

Manganese Intercalation in Graphene/Ir(111): electronic structure — •Hendrik Vita[1], Stefan Böttcher[1], Yuriy Dedkov[2], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]SPECS Surface Nano Analysis GmbH, Berlin, Germany

Transition metal surfaces are ideal templates for the growth of high

quality graphene films. The system graphene/Ir(111) shows rather weak interaction between substrate and the graphene layer. It is well known that transition metals such as Ni and Co, intercalated under graphene/Ir(111), show a rather strong interaction with graphene, yielding massive modifications of the graphene π-band. The intercalation of Mn thin films underneath graphene seems interesting in this context, since Mn has a half filled 3d shell, and the graphene sheet may act as an inert, passivating cover. Here we investigate graphene/Mn/Ir(111) by deposition on top of graphene/Ir(111), and follow the intercalation process by annealing at moderate temperatures using XPS. Investigating the band structure by high resolution ARPES, the Dirac cone is preserved, and we observe a trigonal suppression of the replica Dirac cones, probably due to an enhanced corrugation of the graphene film. A totally different situation occurs if the intercalation process is performed at much higher temperatures. Drastic changes in the band structure emerge, with a shifted π-band to higher binding energies, and a chemical shift of the C1s core level. Additionally, a restructuring of the intercalated Mn thin film is observed by LEED.

TT 97.3 Thu 11:00 MA 041

Atomically Resolved Graphitic Surfaces in Air by Atomic Force Microscopy — •Daniel S. Wastl, Alfred J. Weymouth, and Franz J. Giessibl — University of Regensburg, Universitätsstrasse 31, 93053 Regensburg, Germany

Imaging at the atomic scale with atomic force microscopy in biocompatible environments is an ongoing challenge. We demonstrate here atomic resolution of graphite and hydrogen-intercalated graphene on SiC in air1. The main challenges arise from the overall surface cleanliness and the water layers which form on almost all surfaces2. To further investigate the influence of the water layers, we compare data taken with a hydrophilic bulk-silicon tip to a hydrophobic sapphire tip. While atomic resolution can be achieved with both tip materials at moderate interaction forces, the strong differences in force versus distance spectra can be related to the water layers on the tips and samples. Imaging at very low tip-sample interaction forces results in the observation of large terraces of a naturally-occurring stripe structure on the hydrogen intercalated graphene[1]. This structure has been previously reported on graphitic surfaces that are not covered with disordered adsorbates in ambient conditions (i.e. on graphite and bilayer graphene on SiC[3], but not on monolayer graphene on SiC). Both these observations indicate that hydrogen-intercalated graphene is close to an ideal graphene sample in ambient environments.

[1] Wastl, Weymouth, Giessibl, ACS Nano 8, 5233 (2014).
[2] Wastl Weymouth, Giessibl, Phys. Rev. B 87, 245415 (2013).
[3] Wastl et al., ACS Nano 7, 10032 (2013).

TT 97.4 Thu 11:15 MA 041

A route to free-standing graphene by removal of the Ni substrate by a gas phase reaction — •Ann-Kathrin Henss[1], Patrick Zeller[1], Michael Weinl[2], Matthias Schreck[2], and Joost Wintterlin[1] — [1]Ludwig-Maximilians-Universität, Munich, Germany — [2]Universität Augsburg, Augsburg, Germany

An essential step for the use of graphene in electronic devices is the removal of the underlying metal substrate after graphene growth. We have tested a new route to free-standing graphene grown on thin single crystalline Ni(111) films. The 150 nm thick metal films were epitaxially grown on a Si(111) wafer separated by a 120 to 150 nm thick yttria-stabilized zirconia (YSZ) buffer layer. Aligned monolayer graphene was grown by chemical vapor deposition using ethylene as precursor gas under ultra high vacuum conditions. The graphene quality was monitored by scanning tunneling microscopy and low energy electron diffraction. The subsequent removal of the nickel substrate was performed in a pure gas phase reaction. In the so called Mond process, a chemical transport reaction, nickel reacts with carbon monoxide to gaseous nickel tetracarbonyl at 350 K. By applying a temperature gradient in the reaction furnace the formed carbonyl complex is transported to areas with higher temperature leaving graphene on the isolating YSZ buffer layer of the substrate. X-ray photoelectron spectroscopy, scanning electron microscopy and Raman spectroscopy were used to study the samples after this process.

TT 97.5 Thu 11:30 MA 041

Freestanding lateral nanostructures of two-dimensional carbon materials — •Andreas Winter[1], Yasin Ekinci[2], Rainer Stosch[3], Thomas Weimann[3], Johannes Biskupek[4], Ute Kaiser[4], and Andrey Turchanin[1] — [1]Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany — [2]Laboratory for Micro- and Nanotechnology, Paul Scherrer Institut, 5232 Villigen, Switzerland — [3]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [4]Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm, Germany

Two-dimensional (2D) carbon materials like graphene, hexagonal boron nitride or carbon nanomembranes (CNMs) have recently attracted enormous interest due to their potential use in electronics, chemical and biological sensors, nanofilters, hybrid materials etc. Most applications require a lithographic patterning of these 2D materials. Here we present various micro- and nanostructures of graphene and CNMs as well as their in-plane heterostructures fabricated via optical, e-beam and EUV interference lithography. The preparation of these structures on supporting substrates as well as large area freestanding nanomembranes with patterns varying from ca. 100 μm to 50 nm will be shown. Via electron irradiation, graphene and dielectric CNMs can be stitched together, forming electrically heterogeneous ultrathin 2D carbon sheets. We characterize their properties employing X-ray photoelectron and Raman spectroscopy, helium ion microscopy and high-resolution TEM.

TT 97.6 Thu 11:45 MA 041

Graphene Membranes as Electron Transparent Windows for Photoelectron Spectroscopy — •Jürgen Kraus[1], Robert Reichelt[1], Sebastian Günther[1], Luca Gregoratti[2], Matteo Amati[2], Maya Kiskinova[2], Alexander Yulaev[4], Ivan Vlassiouk[3], and Andrei Kolmakov[4] — [1]TU München Chemie Department, Lichtenbergstr. 4, D-85748 Garching — [2]Sincrotrone Trieste, Area Science Park, 34149 Trieste, Italy — [3]Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — [4]Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899, USA

The high mechanical stability of graphene (g) allows the construction of ultrathin gas tight membranes. Transferred few layer thick g covering the orifice of an environmental cell could be used to seal a water droplet inside the cell from the surrounding vacuum of the ultra-high vacuum chamber into which the cell was introduced. The used membranes were transparent even for slow photoelectrons (PEs), so that the sealed water could be characterized by x-ray photoelectron spectroscopy (XPS). We also measured the electron attenuation length of monolayer g on Cu for PEs of 200-1000 eV kinetic energy. We were able to produce free standing monolayer g by locally electrochemically etching the Cu-substrate underneath the as-grown g. After deposition of gold on the membrane backside and acquiring Au 4f PEs from the opposite site, we proved that $< 1\%$ of a monolayer Au can be detected through the suspended g membrane. This pushes the applicability of our membrane based XPS technique towards surface characterization under ambient conditions.

TT 97.7 Thu 12:00 MA 041

Irradiation of Graphene-FETs with highly charged Ions — •Philipp Ernst[1], Roland Kozubek[1], Oliver Ochedowski[1], Jens Sonntag[2], Axel Lorke[2], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, AG Schleberger, Duisburg, Germany — [2]Universität Duisburg-Essen, AG Lorke, Duisburg, Germany

We have studied the influence of ion bombardment on the properties of graphene field-effect transistor (FET) structures. We used highly charged ions (HCI) with different potential energies at roughly the same kinetic energy (charge state Xe^{32+} and Xe^{25+} with $E_{kin} = 220$ keV and $E_{kin} = 195$ keV). Electrical transport measurements, Raman spectroscopy, and atomic force microscopy were used to investigate the electrical and structural modifications of the graphene-FETs induced by the ion irradiation. The electrical analysis was performed *in-situ* in the ultra-high vacuum set up used for the irradiation. For all investigated fluences, the experiments show a reduction of the mobility, which scales with the potential energy of the ions. Remarkably, the influence of the impact of highly charged ions is already measurable at extremly low fluences < 15 ions/μm^2. As a consequence of the irradiation, a p-doping effect could be observed. Further experiments at lower kinetic energies (< 50 keV) are planned to clarify how the potential energy of the impinging HCIs will affect the observed irradiation effects in graphene.

TT 97.8 Thu 12:15 MA 041

Increasing the mobility of holes in graphene FETs by irradiation with swift heavy ions — •Tobias Foller, Philipp Ernst, Oliver Ochedowski, Roland Kozubek, Lukas Madauss, and Marika Schleberger — Fakultät für Physik and CeNIDE, Uni-

versität Duisburg-Essen, 47048 Duisburg, Germany

In this work graphene field-effect transistors (FETs) are modified by irradiation with swift heavy ions (SHI, Xe^{23+} with $E_{kin} = 91$ MeV). Graphene FETs are prepared by exfoliation of a HOPG crystal followed by deposition of metal contacts via Photolithography. They allow to investigate the mobility of charge carriers in graphene. Current measurements, Raman spectroscopy and atomic force microscopy have been used to investigate the electrical and structural modifications of graphene due to the ion irradiation. By irradiation with swift heavy ions under perpendicular incidence with small fluences (≈ 2500 ions/μm^2), we have succeeded in almost doubling the mobility of holes compared to the unirradiated sample.On the other hand irradiation under glancing incidence ($\leq 2°$) with fluences of 10 ions/μm^2 have revealed that, despite the rather small changes in the (I_D/I_G)-ratio in the Raman spectrum, the charge carrier mobility is significantly reduced.

TT 97.9 Thu 12:30 MA 041

Structure, strain distribution and energetics of basal-plane dislocations in bilayer graphene — •Konstantin Weber and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

A recent TEM study [1] demonstrated that substrate-grown graphene bilayers are typically not perfect in registry, but contain a high concentration of basal-plane dislocations. Using atomistic simulations based on the registry-dependent potential of Kolmogorov and Crespi [2] and the classical AIREBO potential we investigated the atomic structure and the properties of the 4 different types of dislocations with shortest possible Burgers vector in bilayer graphene, the thinnest imaginable crystal that can host such 1D defects. We find that each of the 4 different dislocations splits into two partial dislocations. The partials are equally spaced due to the absence of a stacking fault energy, a peculiar property of bilayer graphene. Furthermore, partials with a step component give rise to a pronounced buckling of the graphene bilayer. An analysis of the atomic structure, local strain distribution, disregistry and dislocation energy of the dislocations will be given and we will highlight how their properties differ from textbook examples of dislocations in 3D crystals.

[1] B.Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H.B. Weber, B. Meyer, E. Spieker, *Nature* **505**, 533 (2014).
[2] A. Kolmogorov, V. Crespi, *Phys. Rev. B* **71**, 235415 (2005).

TT 97.10 Thu 12:45 MA 041

Plasma-enhanced chemical vapor deposition of graphene on metallic substrates — •Nicolas Wöhrl[1], Oliver Ochedowski[2], Steven Gottlieb[2], Stephan Schulz[1], and Volker Buck[2] — [1]Faculty of Chemistry and CENIDE, University Duisburg-Essen, 47057 Duisburg, Germany — [2]Faculty of Physics and CENIDE, University Duisburg Essen, 47057 Duisburg, Germany

In this work we present the synthesis of graphene on copper and nickel substrates by microwave Plasma-enhanced Chemical Vapor Deposition (PE-CVD) process. The special construction of the plasma source allows the deposition at a wide range of different process parameters giving a fast and inexpensive method to synthesize graphene. Additional advantages of the plasma deposition of graphene are lower substrate temperatures compared with thermal CVD processes. In contrast to the thermal CVD the gaseous precursors are already decomposed in the plasma and the plasma parameters are varied to investigate the influence on the nucleation and growth of graphene and on the defect density in the graphene layers. Optical emission spectroscopy is used to characterize the plasma properties while Raman spectroscopy and AFM measurements are used as nondestructive tools for the characterization of the synthesized graphene films. Especially Raman spectroscopy is used as a suitable tool to determine the number of graphene layers, the disorder and the defect density. We present a possible way to produce large area of monolayer graphene on metallic substrates with the prospect to make graphene available for industrial applications.

TT 98: Focus Session: Visualization of Heavy Fermion Formation through Scanning Tunneling Microscopy

Heavy fermion systems owe their name to a narrow band of heavy quasiparticles formed at the Fermi energy as a consequence of the Kondo effect and the consecutive lattice coherence of the Kondo quasiparticle states at low temperatures. The appearance of quantum coherence in the heavy fermion state as well as its instability and/or competition with magnetic ordering can give rise to a wealth of exotic phenomena, ranging from Kondo insulating behavior to quantum phase transitions, Fermi liquid breakdown and to superconductivity. The way how the quantum coherence emerges has been discussed controversially.

Recent progress in achieving low temperatures and sample preparation has established scanning tunneling microscopy (STM) and spectroscopy (STS) as an important new tool for detailed investigation of heavy fermion systems. As specific capabilities of STM, coherence can be probed by interference of different tunneling channels, and the magnetic coupling strength can be tuned by controling the geometry of model systems at metallic surfaces. The Focus Session will discuss these recent developments and prospects for understanding this enigmatic state of matter.

Organizers: Stefan Kirchner (Center for Correlated Matter, Hangzhou) and Johann Kroha (Uni Bonn)

Time: Thursday 15:00–18:15 Location: H 0104

Invited Talk TT 98.1 Thu 15:00 H 0104

Scanning Tunneling Spectroscopy: a New Tool for Probing Heavy Fermion Materials — •Piers Coleman — Department of Physics and Astronomy, Rutgers University, 136 Frelinghuysen Road, Piscataway, NJ 08854, USA — Department of Physics, Royal Holloway, University of London, Egham, Surrey TW20 0EX, UK

Over the past twenty years, the use of Scanning Tunneling Microscopy (STM) has emerged as a powerful tool for imaging the position dependent electronic excitation spectrum of correlated electron materials. More recently, this tool has been applied with great success to heavy electron metals, superconductors and Kondo insulators. Unlike one band materials, such as cuprate superconductors, STM into heavy fermion systems usually involves an interference between tunneling into the conduction d-band and the almost localized f-states, leading to Fano line-shape interference. I shall review the progress in this field, giving particular discussion of the insights gained into the hidden order in URu_2Si_2, the superconductivity in $CeCoIn_5$ and the topological Kondo insulator, SmB_6.

Topical Talk TT 98.2 Thu 15:30 H 0104

The Single-Atom Kondo Effect as a Local Probe for Magnetic Interactions — •Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The Kondo effect of single magnetic atoms adsorbed to metal surfaces induces a zero-bias feature in spectra of the differential conductance acquired with a scanning tunnelling microscope. From the resonance line shape information on the interaction of the magnetic impurity with its local environment may be deduced. Embedding a single Co atom in artificially fabricated clusters of several Cu atoms leads to pronounced changes in the line shape of the Abrikosov-Suhl-Kondo

resonance. Similar hybridization effects occur in single-atom junctions comprising non-magnetic as well as magnetic tips and a single Kondo atom. The distance-dependent magnetic interaction between two Co atoms has been explored in linear $CoCu_nCo$ clusters.

Financial support by the Deutsche Forschungsgemeinschaft through SFB 668 and KR 2912/7-1 is acknowledged.

Topical Talk TT 98.3 Thu 16:00 H 0104

Correlated Electrons under the Microscope: from Atomic Scale Model Systems to Bulk Materials — •Peter Wahl — SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, KY16 9SS, United Kingdom

The physics of strongly correlated and heavy fermion materials is often governed by a delicate balance between magnetic order and screening of magnetic moments. Therefore it is not surprising that some of the key features of the phase diagrams of these materials can be observed already in model systems consisting of two impurities or a chain of impurities. Specifically the two impurity Kondo problem has been theoretically shown to exhibit a quantum phase transition between an antiferromagnetic singlet state and a Kondo screened phase. I will show experiments by low temperature scanning tunnelling microscopy (STM) and spectroscopy for few impurities at surfaces which aim at mimicking these model systems, specifically a realization of the two-impurity Kondo model allowing for continuous tuning of the coupling between the two magnetic atoms by attaching one of the Kondo impurities to the tip of the STM. Attaching magnetic atoms from the surface to the tip of the STM is finally shown to allow for imaging of magnetic structure in strongly correlated electron systems at the atomic scale.

15 min. break.

Topical Talk TT 98.4 Thu 16:45 H 0104

Developing Kondo Lattice Coherence and Quantum Criticality in $YbRh_2Si_2$ — •Steffen Wirth[1], Silvia Seiro[1], Stefan Kirchner[2], Cornelius Krellner[3], Christoph Geibel[1], Qimiao Si[4], and Frank Steglich[1] — [1]MPI for Chemical Physics of Solids, Dresden, Germany — [2]MPI for Physics of Complex Systems, Dresden, Germany — [3]Goethe University Frankfurt, Germany — [4]Rice University, Houston, Texas, USA

Hybridization is a fundamental concept in strongly correlated electron physics. In heavy fermion metals, it may result in the generation of low-energy scales that can give rise to quantum criticality and unconventional superconductivity. An important techniques that helped shaping our understanding of nonlocal correlations – magnetic and superconducting – has been tunneling spectroscopy (STS) with its unique ability to give local, microscopic information that directly relates to the one-particle Green's function. We investigated $YbRh_2Si_2$, an archetypal heavy fermion metal. Quantum criticality is discussed in terms of an antiferromagnetic instability and a Kondo break-down of the heavy quasiparticles. STS studies identified a hybridization-induced gap-like feature of the tunneling conductance. Here we focus on the evolution of the Kondo lattice. While the Kondo lattice starts forming already at the single-ion Kondo temperature, lattice Kondo effects dominate only at much lower temperatures. This establishes a hierarchy of energy scales. Finite-temperature signatures of the QCP are observed in field-dependent STS. Our findings are augmented by band structure calculations and transport measurements.

Invited Talk TT 98.5 Thu 17:15 H 0104

Visualizing the Formation and Magnetically-Mediated Cooper Pairing of Heavy Fermions — •JC Seamus Davis — Cornell University, Ithaca, NY 14850, USA

We recently introduced spectroscopic imaging STM to the study of heavy fermions and achieved the first heavy-quasiparticle interference imaging and direct observation of splitting of a light k-space band into two new heavy fermion bands due to the hybridization process (Nature **465**, 570 (2010)). Key specifics of the Cooper pairing mechanism are encrypted in the k-space structure of the superconducting energy gaps $\Delta_{\alpha,\beta}(k)$ on the heavy bands $E(k)_{\alpha,\beta}$. With energy scales for both these effects so low (sub meV), it was impossible to directly measure $\Delta(k)$ for any heavy-fermion superconductor. We introduced Bogoliubov quasiparticle interference (QPI) imaging using milli-Kelvin STM for $CeCoIn_5$. The heavy band structure $E(k)_{\alpha,\beta}$, the Fermi surface, plus the superconducting $\Delta_{\alpha,\beta}(k)$ structure were measured directly for the first time (Nature Physics **9**, 458 (2013)). Novel SI-STM techniques to measure the k-space structure of the f-electron magnetic interactions were introduced for $CeCoIn_5$. Solving the superconducting gap equations on the measured $E(k)_{\alpha,\beta}$ with the hypothesis that these magnetic interactions mediate the Cooper pairing, reveals succession of quantitative predictions about the superconducting state. We established excellent quantitative agreement between these diverse predictions and many measured characteristics of $CeCoIn_5$. This provides the first direct evidence that its heavy fermion Cooper pairing is mediated by the f-electron magnetism. (PNAS **111**, 11663 (2014))

TT 98.6 Thu 17:45 H 0104

Single-Co Kondo effect on Au(110) — •Stefan Meierott, Nicolas Néel, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

Scanning tunneling spectra of the differential conductance acquired atop single Co atoms on Au(110) exhibit a zero-bias resonance. This feature is attributed to the spectroscopic signature of the Kondo effect. Spatially resolved spectroscopy unveils a mismatch between the maximum resonance amplitude and the Co center. Based on currently available theory [1] the experimental observations are reproduced by taking the adsorption of Co on the facet of a Au(110) missing row into account.

Financial support by the Deutsche Forschungsgemeinschaft through KR 2912/7-1 is acknowledged.

[1] M. Plihal et. al., Phys. Rev. B 63, 085404 (2001)

TT 98.7 Thu 18:00 H 0104

Scanning tunneling spectroscopy and surface quasiparticle interference in models for the topological Kondo insulator SmB_6 — •Pier Paolo Baruselli and Matthias Vojta — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

SmB_6 is one of the candidate compounds for topological Kondo insulators, a class of materials which combines a non-trivial topological band structure with strong electronic correlations. We present a theoretical study [1] of the surface-state signatures induced by dilute impurities in scanning tunneling spectroscopy and quasiparticle interference. We employ a multiband tight-binding description, supplemented by a slave-particle approach to account for strong interactions. We discuss the spin structure of the three surface Dirac cones and provide concrete predictions for the energy and momentum dependence of the resulting QPI signal. Moreover, we analyse the effect of a 2x1 surface reconstruction on such signals.

[1] P. P. Baruselli and M. Vojta, PRB 90, 201106(R) (2014)

TT 99: Superconductivity: (General) Theory 2

Time: Thursday 15:00–18:00 Location: H 2053

TT 99.1 Thu 15:00 H 2053

Functional Development in Density Functional Theory for Superconductors — •Antonio Sanna, E.K.U. Gross, and Frank Essenberger — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

Density functional theory for superconductors (SCDFT) is a fully parameter-free approach to superconductivity that allows for accurate predictions of critical temperature and properties of superconductors. We report on the most recent extensions of the method, in particular the development of new functionals to:

1) incorporate in a correct fashion Migdal's theorem;
2) compute the excitation spectrum;
3) include spin-fluctuation mediated pairing

Applications and predictions are shown for a set of materials, including conventional and unconventional superconductors.

TT 99.2 Thu 15:15 H 2053

Coulomb interaction in Eliashberg theory of Superconductivity — •Arkadiy Davydov, Antonio Sanna, Sangeeta Sharma, John Kay Dewhurst, and Eberhard Gross — Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany

The Eliashberg theory [1] of superconductivity allows to describe materials with strong pairing interaction. In the non magnetic case it leads to a system of coupled integral multidimensional equations. Computational costs are usually reduced by an isotropic limit [2], and by restricting the Coulomb interaction to the use of one single parameter, μ^*, often chosen to give the experimental Tc. In this work we present the parameter-free approach in which the screened Coulomb interaction fully accounted within the Random Phase Approximation, entering the Eliashberg's equations on the same footing as the phononic interaction. We will compare this approach with Density Functional Theory for Superconductors [3, 4] where the corresponding approximation leads to a good agreement with experiments.

[1] G.M. Eliashberg, Sov. Phys. JETP 11, 696 (1960).
[2] D.J. Scalapino, Phys. Rev. 148, 263 (1966).
[3] L.N. Oliveira, E.K.U. Gross, Phys. Rev. Lett. 60, 2430 (1988).
[4] M. Lüders, PRB 72, 024545 (2005).

TT 99.3 Thu 15:30 H 2053

Superconductivity in intercalated group-IV honeycomb structures — •Jose A. Flores Livas and Antonio Sanna — Max-Planck-Institut für Mikrostrukturphysik. Weinberg 2, 06120. Halle (Saale) Germany.

We present in this talk a theoretical investigation on electron-phonon superconductivity of honeycomb MX_2 layered structures. Where X is one element of the group-IV (C, Si or Ge) and M an alkali or an alkaline-earth metal. Among the studied compositions we predict a T_c of 7 K in $RbGe_2$, 9 K in $RbSi_2$ and 11 K in SrC_2. Our SCDFT calculations evidence a strongly anisotropic superconducting gap, and the results show that despite the different doping and structural properties, the three families of materials fall into a similar description of its superconducting behavior. This allows us to estimate an upper critical temperature of about 20 K for the class of intercalated group-IV structures, including intercalated graphite and doped graphene.

TT 99.4 Thu 15:45 H 2053

Tuning non-equilibrium superconductors with lasers — •Michael A. Sentef[1], Alexander F. Kemper[2], Antoine Georges[3], and Corinna Kollath[1] — [1]HISKP, University of Bonn, Nussallee 14-16, D-53115 Bonn, Germany — [2]LBL Berkeley, USA — [3]Ecole Polytechnique and College de France, Paris, France

The study of the real-time dynamics dynamics of solids perturbed by short laser pulses is an intriguing opportunity of ultrafast materials science. Previous theoretical work on pump-probe photoemission spectroscopy revealed spectroscopic signatures of electron-boson coupling [1, 2], which are reminiscent of features observed in recent pump-probe photoemission experiments on cuprate superconductors [3, 4]. Here we investigate the ordered state of electron-boson mediated superconductors subject to laser driving using Migdal-Eliashberg theory on the Kadanoff-Baym-Keldysh contour. We extract the characteristic time scales on which the non-equilibrium superconductor reacts to the perturbation, and their relation to the coupling boson and the underlying order.

[1] M. Sentef et al., Phys. Rev. X 3, 041033 (2013).
[2] A. F. Kemper et al., Phys. Rev. B 90, 075126 (2014).
[3] J. Graf et al., Nat. Phys. 7, 805 (2011);
W. Zhang et al., Nat. Comm. 5, 4959 (2014).
[4] J. D. Rameau et al., Phys. Rev. B 89, 115115 (2014).

TT 99.5 Thu 16:00 H 2053

Conformal phase transition as a new perspective on conventional superconductors — •Flavio Nogueira[1] and Asle Sudbo[2] — [1]Theoretische Physik III, Ruhr-Universität Bochum — [2]Dept. of Physics, Norwegian University of Science and Technology

We argue that the phase transition in strong type I superconductors features charged fluctuations, meaning that it is essentially driven by thermal fluctuations of the magnetic field. This is simply a consequence of the small value of the Ginzburg parameter in the deep type I regime. We substantiate this conclusion by a generalization of the Ginzburg criterion to include charged fluctuations. Finally, we demonstrate by means of a renormalization group analysis that the correlation length actually does not obey a power law as function of $T - T_c$. Rather it features an essential singularity at T_c, which is characteristic of a so called conformal phase transition, one known example of it being the Berezinski-Kosterliz-Thouless (BKT) phase transition in two-dimensional superfluids. We argue that a similar behavior happens in three-dimensional strongly type I superconductors. One important prediction from our theory that may be tested experimentally by microwave measurement is a universal discontinuous jump in the superfluid density.

TT 99.6 Thu 16:15 H 2053

Surface instability of nodal noncentrosymmetric superconductors — •Carsten Timm[1], Stefan Rex[2], and Philip M. R. Brydon[3] — [1]Institute of Theoretical Physics, Technische Universität Dresden, Germany — [2]Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway — [3]Condensed Matter Theory Center, The University of Maryland, College Park, U.S.A.

It has been proposed that nodal noncentrosymmetric superconductors show flat bands of zero-energy surface states [1,2]. Such surface states would realize a two-dimensional gas of Majorana fermions with interesting properties. However, the proposal was based on the assumption that the superconducting gaps assume constant bulk values even in the presence of a surface. We here employ self-consistent mean-field theory to calculate the gaps and the surface states for a slab of finite thickness. We find two phase transitions upon lowering the temperature: At a higher temperature T_c, the slab becomes superconducting and develops flat surface bands. At a lower temperature T_s, time-reversal invariance is spontaneously broken in the surface region and the surface bands become dispersive and are pushed away from the Fermi energy.

[1] A. P. Schnyder and S. Ryu, Phys. Rev. B **84**, 060504(R) (2011).
[2] P. M. R. Brydon, A. P. Schnyder, and C. Timm,
Phys. Rev. B **84**, 020501(R) (2011).

TT 99.7 Thu 16:30 H 2053

Collective modes in superconductors without inversion symmetry — •Nikolaj Bittner[1], Dietrich Einzel[2], Ludwig Klam[1], and Dirk Manske[1] — [1]Max–Planck–Institut für Festkörperforschung, D–70569 Stuttgart, Germany — [2]Walther–Meißner–Institut für Tieftemperaturforschung, D–85748 Garching, Germany

The collective modes characteristic of conventional and unconventional superconductors include the Anderson–Bogoliubov (or gauge) mode ω_G as well as the condensate plasma mode ω_P, to which the gauge mode gets shifted as a consequence of the Anderson–Higgs mechanism (AHM). A unique property of non–centrosymmetric superconductors (ncs) is the coexistence of spin–singlet (Δ_s) and triplet (Δ_{tr}) energy gaps. In the limit of strong spin–orbit coupling there arises a two–band (two–gap) structure, which automatically implies the existence of a new massive collective mode ω_L, discovered by A. J. Leggett in 1966 for ordinary two–band superconductors, the so–called Leggett mode. In this contribution we focus on the analysis of the electromagnetic response of the superconducting condensate and specify for the first time the collective modes ω_G, ω_P and ω_L in ncs systems of cubic

and tetragonal symmetry. Particular emphasis is on the analysis of Leggett's collective mode in ncs systems for which we can show that (i) it is, besides the gauge mode, necessary to guarantee charge conservation, (ii) the AHM only slightly modifies its dispersion and leaves its mass unaffected, (iii) it survives in the limit of vanishing triplet admixture $t = \Delta_{tr}/\Delta_s$ to the singlet energy gap and (iv) its form is symmetry–dependent (cubic, tetragonal) for finite triplet admixture t.

15 min. break.

TT 99.8 Thu 17:00 H 2053

The fate of the superconducting gap close to two magnetic Shiba impurities — •Tobias Meng[1,2], Silas Hoffman[2], Jelena Klinovaja[2], and Daniel Loss[2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

As a potential host for Majorana zero energy bound states, chains of magnetic impurities in superconductors are attracting an increasing amount of attention. Working towards a better understanding of the physics of such chains, we address the effect of a single, and of two close magnetic impurities in a superconductor. Specifically, we analytically calculate how the presence of the Cooper pair breaking Shiba impurities locally reduces the superconducting gap. We show that the gap renormalization can favor an antiferromagnetic ordering of the impurities that competes, e.g., with the RKKY exchange.

TT 99.9 Thu 17:15 H 2053

Collective modes in superconducting rhombohedral graphite — •Ville Kauppila[1], Timo Hyart[2], and Tero Heikkilä[2] — [1]O.V. Lounasmaa Laboratory, Aalto University, Finland — [2]University of Jyväskylä, Finland

Recently it was realized that coupling particles with a Dirac dispersion (such as electrons in graphene) can lead to a topologically protected state with flat band dispersion. Such a state could support superconductivity with unusually high critical temperatures[1]. Perhaps the most promising way to realize such coupling in real materials is in the surface of rhombohedrally stacked graphite.

We consider collective excitations (i.e. the Higgs modes) in surface superconducting rhombohedral graphite. We find two amplitude and two phase modes corresponding to the two surfaces of the graphite where the superconductivity lives. We calculate the dispersion of these modes. We also derive the Ginzburg-Landau theory for this material. We show that in superconducting rhombohedral graphite, the collective modes, unlike in conventional BCS superconductors, give a large contribution to thermodynamic properties of the material.

[1] T.T. Heikkila, N.B. Kopnin, G.E. Volovik, Phys. Rev. B 83, 220503(R) (2011)

TT 99.10 Thu 17:30 H 2053

Interaction effects along the edge of a topological superconductor — •Johannes S Hofmann[1,2], Andreas P Schnyder[2], and Fakher Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Würzburg, Deutschland — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Deutschland

Topological nodal superconductors, such as d_{xy}-wave and nodal noncentrosymmetric superconductors, exhibit protected zero-energy flat-band edge states. These zero-energy edge modes are protected by time-reversal and translation symmetry and their stability is guaranteed by the conservation of a quantized topological invariant. Here, we study the fate of these flat-band edge states in the presence of interactions. We find that Hubbard interactions lead to spontaneous breaking of time-reversal or translation symmetry at the edge of the system. For the d_{xy}-wave superconductor in the presence of attractive Hubbard interactions we find that the flat-band states become unstable towards the formation of a charge-density wave state or a state with s-wave type pairing correlations. Repulsive Hubbard interactions, on the other hand, induce ferromagnetic order at the edge of the d_{xy}-wave superconductor.

TT 99.11 Thu 17:45 H 2053

Superconductivity of heavy fermions in the Kondo lattice model — •Steffen Sykora[1] and Klaus W. Becker[2] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany

Understanding of the origin of superconductivity in strongly correlated electron systems is one of the basic unresolved problems in physics. Examples for such systems are the cuprates and also the heavy-fermion metals, which are compounds with $4f$ and $5f$ electrons. In all these materials the superconducting pairing interaction is often believed to be predominantly mediated by spin fluctuations and not by phonons as in normal metals. For the Kondo-lattice model we present results, which are derived within the Projective Renormalization Method (PRM). Based on a recent study of the one-particle spectral function for the normal state we first derive an effective Hamiltonian which describes heavy fermion quasiparticle bands close to the Fermi surface. An extension to the superconducting phase leads to d-wave solutions for the superconducting order parameter in agreement with recent STM measurements.

TT 100: Correlated Electrons: Other Materials

Time: Thursday 15:00–18:30 Location: H 3005

TT 100.1 Thu 15:00 H 3005

The effects of spin-orbit coupling and electron correlations on the Fermi surface of Sr_2RuO_4 — •Guoren Zhang[1], Evgeny Gorelov[1], and Eva Pavarini[1,2] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425, Jülich, Germany — [2]JARA High-Performance Computing

In this work we investigate the effects of spin-orbit coupling (SOC) and electron correlations on the Fermi surface (FS) of Sr_2RuO_4. We first study the spin-orbit coupling effects by comparing the FSs obtained by local-density approximation (LDA) and LDA+SOC calculations. Then, to study the effects of electron correlations, we perform LDA + dynamical mean field theory method (DMFT) and LDA+SOC+DMFT calculations. Our LDA and LDA+SOC results are consistent with previous theoretical works [1, 2]. Our LDA+SOC+DMFT results show that, in order to reproduce the experimental FS [3], it is key to include both effects.

[1] M. W. Haverkort, I. S. Elfimov, L. H. Tjeng, G. A. Sawatzky, and A. Damascelli, Phys. Rev. Lett. **101**, 026406 (2008).
[2] E. Pavarini, and I. I. Mazin, Phys. Rev. B **74**, 035115 (2006).
[3] A. Damascelli, D. H. Lu, K. M. Shen, N. P. Armitage, F. Ronning, D. L. Feng, C. Kim, Z. X. Shen, T. Kimura, Y. Tokura, Z. Q. Mao and Y. Maeno, Phys. Rev. Lett. **85**, 5194 (2000).

TT 100.2 Thu 15:15 H 3005

LDA+DMFT calculation of optical conductivity of layered ruthenates — •Esmaeel Sarvestani, Guoren Zhang, Evgeny Gorelov, and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Juelich, D-52425 Juelich, Germany

Motivated by recent precise measurements of optical conductivity of correlated metals, we have used the LDA+DMFT method to calculate the optical spectra of paradigmatic correlated metals, strontium ruthenate oxides. The optical conductivity calculation is performed via linear response theory and Kubo's formalism.
For single layer ruthenate oxide, calculations are done for various temperatures. The effects of spin-orbit coupling on the optical spectra are studied. Two sets of interaction parameters, Hubbard U and Hund*s coupling J, which are commonly employed for these systems, have been used. It is shown that for smaller value of interaction, spin-orbit coupling does not change the spectra very much. For larger value of interaction, only if spin-orbit coupling is taken into account, the main features of experimental spectra are reproduced.
By means of numerical analysis, the role of spin-orbit coupling in optical conductivity is traced back to specific elements of the self-energy matrix and single particle spectral functions.
Finally, results of conductivity for double layer ruthenate are also presented.

TT 100.3 Thu 15:30 H 3005

On the absence of an orbital-ordering transition in $KCuF_3$ — •Hunter Sims[1], Eva Pavarini[2], and Erik Koch[1] — [1]German Research School for Simulation Sciences, 52428 Jülich, Germany — [2]Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

The Mott insulating perovskite $KCuF_3$ is considered the paradigm of a long-ranged orbitally-ordered material with cooperative Jahn-Teller distortion. We have found, however, that neither the Kugel-Khomskii superexchange mechanism nor the Jahn-Teller effect can, even qualitatively, account for the observed absence of a transition to a symmetric phase at high temperature. Instead, we show that the distortion of the F-octahedra is only limited by the shortest distance between Cu and F, leading to an increased distortion for the thermally expanded material. To quantitatively understand this we calculate the temperature-dependent Born-Oppenheimer surfaces in LDA+U. Based on this we determine the temperature-dependence of the distortion using a generalization of the Halperin-Englman mean-field model.

TT 100.4 Thu 15:45 H 3005

Long-range Coulomb interaction in surface systems: From cRPA to GW+DMFT — •Philipp Hansmann[1,2], Thomas Ayral[1,3], Antonio Tejeda[4], and Silke Biermann[1] — [1]Centre de Physique Theorique, Ecole Polytechnique, CNRS-UMR7644, 91128 Palaiseau, France — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [3]Institut de Physique Theorique (IPhT), CEA, CNRS, URA 2306, 91191 Gif-sur-Yvette, France — [4]Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, 91192 Gif sur Yvette, France

In spectroscopic (ARPES, cPES) and STM experiments group IV adatoms on semiconductors X:Si/Ge(111) (X=Sn, Si, C, Pb) show competing ground states but are partially in strong contradiction with one another. Ab initio derivation of a low energy Hamiltonian, including constrained RPA calculation for the effective interaction, suggests i) that correlation effects are beyond a single particle treatment and ii) an effective interaction which is not of a local "Hubbard U" type, but has a long-range character. Tackling the problem with standard dynamical mean-field methods (DMFT) is, hence, rather questionable. Instead we depart from the local approximation of DMFT to include, fully self-consistently, non-local effects in a GW+DMFT scheme. We observe that the non-local interaction is responsible for (experimentally observed) charge fluctuations which in some materials (Pb:Si/Ge(111), Sn:Ge(111)) are frozen in a commensurate charge order while in others (Sn:Si(111)) they remain dynamic and explain above mentioned experimental controversies.

TT 100.5 Thu 16:00 H 3005

Structural distortions in Vanadium Sesquioxide (V_2O_3) — •Daniel Grieger and Michele Fabrizio — Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy

Vanadium Sesquioxide (V_2O_3) has attracted large attention mainly because of its prototypical Mott insulating behaviour with negative (chemical) pressure/Chromium doping. Besides trying to shed some light on details of this transition, this contribution is primarily aimed at the structural distortions that accompany the electronic phase diagram. These are especially important near the transition to the low-temperature ($T < 140$K) antiferromagnetic insulating phase, as well as in a recently discovered high-pressure monoclinic metallic phase. The relation and concurrence of the former with the antiferromagnetic ordering is investigated theoretically, which also has consequences for the appearance of the high-pressure phase. Formalisms applied for this purpose are combinations of traditional electronic structure formalisms and DFT+-like approaches.

TT 100.6 Thu 16:15 H 3005

Instantaneous Band Gap Collapse in VO_2 caused by Photocarrier Doping — •Marc Herzog[1], Daniel Wegkamp[1], Lede Xian[2,3], Matteo Gatti[3,4], Pierluigi Cudazzo[2,3], Christina L. McGahan[5], Robert E. Marvel[5], Richard F. Haglund[5], Angel Rubio[1,2,3,6], Martin Wolf[1], and Julia Stähler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Univ. del País Vasco, San Sebastian, Spain — [3]European Theoretical Spectroscopy Facility (ETSF) — [4]École Polytechnique, Palaiseau, France — [5]Vanderbilt Univ., Nashville, Tennessee, USA — [6]MPI for the Structure and Dynamics of Matter, Hamburg, Germany

We have investigated the controversially discussed mechanism of the insulator-to-metal transition (IMT) in VO_2 by means of femtosecond time-resolved photoelectron spectroscopy (trPES). Our data show that photoexcitation transforms insulating monoclinic VO_2 quasi-instantaneously into a metal without an 80 fs structural bottleneck for the photoinduced electronic phase transition. First-principles many-body perturbation theory calculations reveal an ultrahigh sensitivity of the VO_2 band gap to variations of the dynamically screened Coulomb interaction thus supporting the fully electronically driven isostructural IMT indicated by our trPES results. We conclude that the ultrafast band structure renormalization is caused by photoexcitation of carriers from localized V $3d$ valence states, strongly changing the screening before significant hot-carrier relaxation or ionic motion has occurred.

TT 100.7 Thu 16:30 H 3005

Spinon Confinement in the Quasi-1D Ising-like Antiferromagnet $SrCo_2V_2O_8$ — •Zhe Wang[1], Michael Schmidt[1], Anup Kumar Bera[2], Bella Lake[2,3], Alois Loidl[1], and Joachim Deisenhofer[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [3]Institut für Festkoerperphysik, Technische Universität Berlin, Berlin, Germany

Using THz transmission spectroscopy in magnetic field, we have investigated low-energy magnetic excitations in the quasi-one-dimensional Ising-like XXZ antiferromagnet $SrCo_2V_2O_8$. Spinon-pair excitations on the antiferromagnetic ground state have been observed in the XXZ antiferromagnet. Spinon-pair bound states with entangled spin-orbit moment S = 1 are determined unambiguously. The hierarchy of the spinon-pair boundstates can be described by a one-dimensional Schrödinger equation with a linear confinement potential imposed by the interchain interaction.

15 min. break.

TT 100.8 Thu 17:00 H 3005

The influence of the phosphor z position on the Fermi surface of $SrCo_2P_2$: Experiment and theory. — •K. Götze[1,2], J. Klotz[1,2], C. Bergmann[3], C. Geibel[3], H. Rosner[3], I. Kraft[3], V. Lorenz[4], and J. Wosnitza[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Max-Planck-Institut CPfS, Dresden, Germany — [4]IFW, Dresden, Germany

The exact crystallographic and electronic structure plays an important role for the occurrence of quantum criticality, magnetic order, and superconductivity in the family of transition-metal pnictides AT_2Pn_2. The pnictide-distance z is a crucial parameter for the electronic structure because the distance between the T_2Pn_2 layers determines whether the tetragonal crystal structure is collapsed or uncollapsed and, thereby, whether pnictide bonds are formed or not.

We have investigated the influence of the P z position on the band structure of the strongly enhanced Pauli paramagnet $SrCo_2P_2$, a close relative to the superconducting iron arsenides, that is on the verge of magnetic order. The pronounced temperature dependence of the P z position influences the density of states (DOS) at the Fermi energy strongly. Therefore, we have investigated the Fermi surface of $SrCo_2P_2$ in the paramagnetic ground state with the de Haas-van Alphen effect. We compare our experimental results to band-structure calculations in order to determine the exact contribution of individual orbits to the DOS. We will also address the renormalization of the effective masses and the dimensionality of the Fermi surface.

TT 100.9 Thu 17:15 H 3005

Angle-resolved photoemission spectroscopy of correlated electron pairs on NiO and CoO — •Michael Huth[1], Cheng-Tien Chiang[1,2], Andreas Trützschler[1,2], Wolf Widdra[2,1], Jürgen Kirschner[1,2], and Frank O. Schumann[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120, Halle(Saale), Germany — [2]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120, Halle(Saale), Germany

It is well received that the independent electron approximation breaks down in strongly correlated materials. Therefore there is a keen interest to develop a direct experimental probe to spectroscopically resolve the characteristic feature of electron correlation in those materials. One way is to explore double photoemission (DPE) where an electron pair is emitted by a single photon. We use a laboratory high-order harmonic generation light source and the electrons are detected in co-

incidence with a pair of time-of-flight spectrometers operated in an angle resolving mode [1]. We present DPE spectra from the valence band of strongly correlated 3d transition metal oxides such as NiO and CoO films and characterize the two-dimensional energy and momentum distributions of the photoelectron pairs. Possible signatures of the electron correlation will be discussed.

[1] Huth, Chiang, Trützschler, Schumann, Kirschner, Widdra, Appl. Phys. Lett. 104, 061602 (2014)

TT 100.10 Thu 17:30 H 3005

Ground state oxygen holes and the metal-insulator transition in rare earth nickelates — •Thorsten Schmitt[1], Valentina Bisogni[1], Sara Catalano[2], Marta Gibert[2], Raoul Scherwitzl[2], Yaobo Huang[1], Vladimir Strocov[1], Pavlo Zubko[2], Robert J. Green[3], Shadi Balandeh[3], George Sawatzky[3], and Jean-Marc Triscone[2] — [1]Research Department Synchrotron Radiation and Nanotechnology, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [2]Département de Physique de la Matière Condensée, University of Geneva, Switzerland — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada

Perovskite rare-earth (Re) nickelates $ReNiO_3$ continue to attract a lot of interest owing to their intriguing properties like a sharp metal to insulator transition (MIT), unusual magnetic order [1] and expected superconductivity in specifically tuned super-lattices [2]. Full understanding of these materials, however, is hampered by the difficulties in describing their electronic ground state (GS). From X-ray absorption (XAS) at the Ni $2p_{3/2}$ edge of thin films of $NdNiO_3$ and corresponding RIXS maps vs. incident and transferred photon energies we reveal that the electronic GS configuration of $NdNiO_3$ is composed of delocalized and localized components. Our study conveys that a Ni $3d^8$-like configuration with holes at oxygen takes on the leading role in the GS and the MIT of $ReNiO_3$ as proposed by recent model theories [3].

[1] Medarde et al., J. Phys. Cond. Matt. 9, 1679 (1997).
[2] Chaloupka et al., PRL 100, 016404 (2008).
[3] Mizokawa et al., PRB 61, 11263 (2000);
Park et al., PRL 109, 156402 (2012).

TT 100.11 Thu 17:45 H 3005

Correlation driven charge and spin fluctuations in $LaCoO_3$ — •Michael Karolak[1], Manuel Izquierdo[2,3,6], Serguei L. Molodtsov[2,4,5], and Alexander I. Lichtenstein[6] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]European XFEL GmbH, Albert-Einstein-Ring 19, 22761 Hamburg, Germany — [3]Synchrotron Soleil, L'Orme des Merisiers St-Aubin, BP-48, 91192, Gif-sur-Yvette, France — [4]Institute of Experimental Physics, Technische Universität Bergakademie Freiberg, 09599 Freiberg, Germany — [5]ITMO University, Kronverkskiy pr. 49, 197101 St. Petersburg, Russia — [6]Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany

The spin transition in $LaCoO_3$ has been investigated within the DFT+DMFT formalism using continuous time quantum Monte Carlo. Calculations on the experimental rhombohedral atomic structure with two Co sites per unit cell show that an independent treatment of the Co atoms results in a ground state with charge imbalance induced by electronic correlations. Each atom shows a contribution from either a d^5 or a d^7 state in addition to the main d^6 state. These charged states play a relevant role in the spin transition which can be understood as a low spin-high spin (LS-HS) transition with significant contributions ($\sim$ 10%) to the LS and HS states of d^5 and d^7 states. A thermodynamic analysis reveals that the introduction of charge imbalance significantly lowers the total energy of the system.

TT 100.12 Thu 18:00 H 3005

Electronic and magnetic properties of manganese pnictides — •Manuel Zingl, Simon Erker, and Markus Aichhorn — Institute of Theoretical Physics and Computational Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

We study the electronic and magnetic properties of the manganese based compounds $BaMn_2As_2$ and LaOMnAs by combining density functional theory and dynamical mean field theory (DFT + DMFT). These systems crystallize in the same structure as the iron based pnictide superconductors and were experimentally determined to small gap semiconductors with a Néel type antiferromagnetic ground state. With our study we will clarify the importance of electronic correlations on the formation of the insulating gap. Within DMFT we consider a dp-model corresponding to the experimental crystal structure and we investigate the influence of the selected energy window, the double counting correction and the interaction parameters U and J.

TT 100.13 Thu 18:15 H 3005

Pressure-induced semimetal to semiconductor transition in bismuth. — •Konstantin Semeniuk, Philip Brown, Aleksandar Vasiljkovic, and Malte Grosche — University of Cambridge, Cambridge, The United Kingdom

The semimetal bismuth stands out among the elements for its extremely low carrier concentration. This arises from small electron and hole Fermi surface pockets, which amount to about 10^{-5} of the Brillouin zone, or one mobile electron per 100,000 atoms. Situated very close to the transition to a semiconductor, the electronic structure can be tuned further by doping with antimony or by applied hydrostatic pressure.

We investigate the electrical resistivity, Hall effect and Shubnikov de Haas oscillations of single crystal bismuth under hydrostatic pressure of up to 25 kbar in a piston cylinder pressure cell. While the temperature dependence of the resistivity is metallic at ambient pressure, it develops a pronounced kink and subsequently a maximum near 40 K with increasing pressure. The maximum shifts towards lower temperature with further increasing pressure until, above about 20 kbar, the resistivity of bismuth resembles that of a narrow-gap semiconductor. These results suggest that the Lifshitz transition from semimetal to semiconductor can indeed be studied in bismuth at pressures less than 25 kbar, at which a structural transition into a fully metallic state takes place. This makes it possible to access ultra-low carrier density states at intermediate pressures, in which the quantum limit can be reached at very low applied fields.

TT 101: Low-Dimensional Systems: Topological Order 2 (jointly with DS, HL, MA, O)

Time: Thursday 15:00–18:30 Location: H 3010

TT 101.1 Thu 15:00 H 3010

Topological entropy in the classical toric code model — •Johannes Helmes and Simon Trebst — Institut für Theoretische Physik, Universität zu Köln, Germany

For interacting quantum many-body systems the study of entanglement entropies is well established to analyze the fundamental nature of their ground states. In particular, the O(1) correction to the prevalent boundary-law can be used to identify topological order. However, not only in quantum systems, but also in classical systems we can track topological contributions to the classical entropy by employing an analogous approach.

We report results for the classical toric code model in a magnetic field which has a topologically protected zero field degeneracy. We show, how the classical entropy tracks the break-down of the classical topological order upon increasing the external field or temperature. In more technical terms, we apply the replica technique to calculate Renyi entropies from classical Monte Carlo simulations using a newly developed update scheme for efficient loop-gas sampling.

TT 101.2 Thu 15:15 H 3010

Symmetry fractionalization in SU(2n) antiferromagnetic Heisenberg chains — •Andreas Weichselbaum[1] and Thomas Quella[2] — [1]Ludwig Maximilians University, Munich, Germany — [2]University of Cologne, Germany

We explore generalizations of the Affleck-Kennedy-Lieb-Tasaki (AKLT, 1987) model for spin-1 antiferromagnetic Heisenberg chains to higher-rank SU(2n) symmetries. In particular we show that by proper tuning of higher order spin interactions there also exist exact low-dimensional matrix-product ground states with fractionalized edge states. These states are adiabatically connected to the ground state of the plain SU(2n) Heisenberg model. The parameter space is explored using state of the art density matrix renormalization group (DMRG),

explicitly utilizing SU(N) symmetry up to N=6 based on the QSpace tensor library.

TT 101.3 Thu 15:30 H 3010

Protection of topological phases by quantum deformed symmetries — •Thomas Quella — Universität zu Köln, Institut für Theoretische Physik, Köln, Germany

We show that topological phases of quantum spin systems may enjoy protection even in the absence of ordinary group symmetries. The relevant mechanism is explained in full detail for the example of 1D spin chains with quantum group (q-deformed) symmetry $SO_q(3)$. We also sketch the generalization to quantum deformations of other continuous Lie groups such as those associated with $SU(N)$ or $SO(N)$. Our results provide a complete classification of quantum group symmetry protected topological phases for real values of q.

TT 101.4 Thu 15:45 H 3010

Topological phase transition in the quench dynamics of a Fermi gas — •Pei Wang — Department of Physics, Zhejiang University of Technology, Hangzhou 310023, China and Institute for Theoretical Physics, University of Goettingen, German

We study the quench dynamics of a one-dimensional ultracold Fermi gas with synthetic spin-orbit coupling. At equilibrium, the ground state of the system can undergo a topological phase transition and become a topological superfluid with Majorana edge states. As the interaction is quenched near the topological phase boundary, we identify an interesting dynamical phase transition of the quenched state in the long-time limit, characterized by an abrupt change of the pairing gap at a critical quenched interaction strength. We further demonstrate the topological nature of this dynamical phase transition from edge-state analysis of the quenched states. Our findings provide interesting clues for the understanding of topological phase transitions in dynamical processes, and can be useful for the dynamical detection of Majorana edge states in corresponding systems.

TT 101.5 Thu 16:00 H 3010

Diagnosing the statistics of excitations from the dynamical structure factor — •Siddhardh Morampudi[1], Ari Turner[2], and Frank Pollmann[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland

We show that the statistics of excitations in quantum spin liquids yield characteristic features in the dynamical structure factor. Quantum spin liquids are exotic phases of matter which fall beyond the traditional paradigm of symmetry breaking. Originally proposed by Anderson with regard to high temperature superconductivity, they are now widely believed to arise in frustrated spin systems such as the antiferromagnetic Heisenberg model on the kagome lattice. Recently, various theoretical methods to characterize spin liquids have been introduced, especially with regard to numerical simulations. In this work, we obtain results connecting the statistics of the excitations to features of the dynamical structure factor which can be obtained from neutron scattering. We furthermore demonstrate how the results can be used to distinguish different types of gapped spin liquids.

TT 101.6 Thu 16:15 H 3010

Dissipative Chern Insulators — •Jan Carl Budich[1,2], Peter Zoller[1,2], and Sebastian Diehl[3] — [1]Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria — [2]Institute for Quantum Optics and Quantum Information, Austrian Academy of Sciences, 6020 Innsbruck, Austria — [3]Institute of Theoretical Physics, TU Dresden, D-01062 Dresden, Germany

Engineered dissipation can be employed to prepare interesting quantum many body states in a non-equilibrium fashion. The basic idea is to obtain the state of interest as the unique steady state of a quantum master equation, irrespective of the initial state. Due to a fundamental interference of topology and locality, the dissipative preparation of gapped topological phases with a non-vanishing Chern number has so far remained elusive. Here, we study the open quantum system dynamics of fermions on a two-dimensional lattice in the framework of a Lindblad master equation. In particular, we discover a novel mechanism to dissipatively prepare a topological steady state with non-zero Chern number by means of short-range system bath interaction. Quite remarkably, this gives rise to a stable topological phase in a non-equilibrium phase diagram. We demonstrate how our theoretical construction can be implemented in a microscopic model that is experimentally feasible with cold atoms in optical lattices.

TT 101.7 Thu 16:30 H 3010

Absence of an interaction driven Chern insulating phase on the honeycomb lattice — •Johannes Motruk, Adolfo G. Grushin, and Frank Pollmann — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Deutschland

Mean field calculations in the literature have suggested the existence of an interaction-induced Chern insulator (CI) phase in a tight-binding model of spinless fermions on a honeycomb lattice with nearest- and next-nearest-neighbor interactions. The CI phase is an example of a state that breaks time-reversal symmetry spontaneously and possesses a quantized Hall conductance. However, it has been proven elusive in exact diagonalization (ED) studies of this system. Since ED is limited to small system sizes, the fate of this phase in the thermodynamic limit still remains unclear. Using the infinite density matrix renormalization group (iDMRG) algorithm we reach system sizes exceeding those accessible in ED calculations while keeping track of quantum fluctuations neglected in mean field studies. We map out the phase diagram as a function of both nearest- and next-nearest-neighbor interaction strengths for an infinite cylinder geometry and find different charge-ordered phases but no sign of the interaction driven Chern insulator phase.

15 min. break.

TT 101.8 Thu 17:00 H 3010

Quasiparticle interference patterns from different impurities on the surface of pyrochlore iridates: signatures of the Weyl phase — •Fabian Lambert[1], Andreas Schnyder[2], Roderich Moessner[3], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [3]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany

Weyl semi-metals exhibit topologically protected surface Fermi arcs, which pairwise connect projections of bulk band touchings in the surface Brillouin zone. The nontrival spin and orbital character of these topological surface states can be tested experimentally using quasiparticle interference (QPI) measurements. Here, we compute the QPI patterns for a Hubbard Hamiltonian on a pyrochlore lattice. For weak impurity potentials, the QPI patterns can be computed within the First Born approximation. To account for the antiferromangetic spin configuration of $R_2Ir_2O_7$, we treat the Hubbard interaction at the mean-field level. In the antiferromagnetic state the quadratic band touching of the model is split into eight linear band touchings, each of which carries a non-trivial Chern number, thereby realizing a Weyl phase with broken time- reversal symmetry. Using exact diagonalization, we compute the surface spectrum and quasiparticle interference patterns of this Weyl phase for various surface impurities. We show that the spin and orbital texture of the surface states can be inferred from the absence of certain backscattering processes and from the symmetries of the QPI features.

TT 101.9 Thu 17:15 H 3010

Interacting surface states of three-dimensional topological insulators — •Titus Neupert[1], Stephan Rachel[2], Ronny Thomale[3], and Martin Greiter[3] — [1]Princeton Center for Theoretical Science, Princeton University, Princeton, New Jersey 08544, USA — [2]Institute for Theoretical Physics, Technische Universitaet Dresden, 01171 Dresden, Germany — [3]Institute for Theoretical Physics, University of Wuerzburg, Am Hubland, D-97074 Wuerzburg, Germany

We numerically investigate the surface states of a strong topological insulator in the presence of strong electron-electron interactions. We choose a spherical topological insulator geometry to make the surface amenable to a finite size analysis. The single-particle problem maps to that of Landau orbitals on the sphere with a magnetic monopole at the center that has unit strength and opposite sign for electrons with opposite spin. Assuming density-density contact interactions, we find superconducting and anomalous (quantum) Hall phases for attractive and repulsive interactions, respectively, as well as chiral fermion and chiral Majorana fermion boundary modes between different phases. Our setup is preeminently adapted to the search for topologically ordered surface terminations that could be microscopically stabilized by tailored surface interaction profiles.

TT 101.10 Thu 17:30 H 3010

Resonant scattering in the topological Dirac semimetal Cd_3As_2 — Vladimir Gnezdilov[1,2], Azat Sharafeev[1], •Peter Lemmens[1], Raman Sankar[3], and Fangcheng Chou[3] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE NAS, Ukraine — [3]CCMS, National Taiwan Univ., Taipei, Taiwan

In the symmetry-broken topological Dirac semimetal with strong spin-orbit coupling, Cd_3As_2, a pronounced temperature evolution of quasielastic electronic Raman scattering and resonant effects are observed. These effects are then compared to observations in topological insulators, as Bi_2Se_3.

Work supported by RTG-DFG 1953/1, Metrology for Complex Nanosystems and the Laboratory for Emerging Nanometrology Braunschweig, TU Braunschweig.

TT 101.11 Thu 17:45 H 3010

Angle-resolved Photoemission Investigation of SmB_6 — •Peter Hlawenka[1], Oliver Rader[1], Konrad Siemensmeyer[1], Eugen Weschke[1], Andrei Varykhalov[1], Natalya Shitsevalova[2], Slavomir Gabani[3], Karol Flachbart[3], and Emile Rienks[1] — [1]Helmholtz-Zentrum Berlin — [2]Institute for Problems of Material Science, Kiev — [3]IEP, Slovak Academy of Science, Kosice

Recently the mixed valence compound SmB_6 has drawn great attention. Theoretically predicted surface states, which should result from a hybridisation of localised f-bands with conduction electrons and a band inversion, would make SmB_6 the first realisation of a so called topological Kondo insulator [1-2]. Conductivity and transport measurements, as well as spin-resolved photoemission spectroscopy seem to fortify the scenario of a topological nature of the conductive surface [3-5]. We investigate the surface electronic structure of SmB_6 by means of high resolution angle-resolved photoemission spectroscopy measurements below 1 K. We will present new insights into the surface states that determine the low temperature conductivity of this material.

[1] Dzero et al., PRL 104, 106408 (2010).
[2] Lu et al., PRL 110, 096401 (2013).
[3] Wolgast, PRB 88, 180405 (2013).
[4] Kim, Sci. Rep. 3, 3150 (3013).
[5] Xu et al., Nat. Com. 5, 4566 (2014).

TT 101.12 Thu 18:00 H 3010

Calculation of topological properties of strongly correlated electrons without inversion symmetry using Wannier charge centres. — •Robert Triebl and Markus Aichhorn — Institute of Theoretical Physics and Computational Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

We study the topological properties of a role model for interacting Z_2 topological insulators, namely the Kane-Mele-Hubbard model including a staggered sublattice potential controlled by a parameter λ_ν, which breaks inversion symmetry. The applicability of a naïve mean field approach was analysed by comparing to a variational cluster approach, employing a two-site dynamical impurity approximation (DIA). The obtained Greens function determines the topological Hamiltonian, which maps the interacting system to an effective free-particle model with the same topological properties. Since inversion symmetry is lost, we calculate the Z_2 invariant for both Mean Field and topological Hamiltonian using Wannier charge centers. We conclude that a two-site DIA in combination with Wannier charge centers is an easy-to-implement and stable method to determine topological invariants for interacting systems. Comparing with mean field results we find that the direction of magnetisation is crucial for topological properties and hence an inherent mean field magnetisation may lead to incorrect results.

TT 101.13 Thu 18:15 H 3010

An analytical study of the entanglement spectrum of graphene bilayers — •Sonja Predin and John Sliemann — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We present an analytical study of the entanglement spectrum of graphene bilayers. The entanglement spectrum has been proposed as a ground state property that exhibits characteristic energy excitations[1]. Futhermore, it was claimed that gapless systems possess the same number of Dirac cones as their entanglement spectrum [2]. In addition, it was suggested that the entanglement spectrum is a promising tool to characterize topological phases. In this work we will show that the energy spectrum of an gapless system and its entanglement spectrum can have a different topology. In particular, we will show that Lifshitz transitions change the topology of the energy spectrum of graphene bilayers in a different way than the topology of entanglement spectrum. The topology of the energy spectrum of graphene bilayers for small energies is changed by Lifshitz transitions by changing the connectivity by the appearance of the three additional Dirac cones around every Dirac point [3]. The entanglement spectrum, on the other hand, is changed by deforming a Dirac cone into a neck characterized by vanishing eigenvalues of the entanglement Hamiltonian.

[1] H. Li and F. D. M. Haldane,
Phys. Rev. Lett. 101, 010504 (2008)
[2] A. M. Turner, et al., Phys. Rev. B, 82, 241102R (2010)
[3] J. Cserti, et al., Phys. Rev. Lett. 99, 066802 (2007)

TT 102: Transport: Quantum Dots, Quantum Wires, Point Contacts 2 (jointly with HL)

Time: Thursday 15:00–18:30 Location: A 053

TT 102.1 Thu 15:00 A 053

Weak antilocalization and spin-orbit interaction in epitaxial nanowires — Brian Tarasinski[1], Ilse van Weperen[2], Debbie Eeltink[2], Vlad Pribiag[2], Erik Bakkers[2,3], Leo Kouwenhoven[2], and •Michael Wimmer[2] — [1]Leiden University, The Netherlands — [2]Delft University of Technology, The Netherlands — [3]Eindhoven University of Technology, The Netherlands

We develop a theory of weak antilocalization for three-dimensional nanowires that allows for a quantitative extraction of spin-orbit strength. To this end we perform numerical Monte Carlo simulations of classical trajectories that are used in the quasiclassical theory of weak antilocalization. In particular, we show that magnetoconductance in three-dimensional nanowires is very different compared to wires in two-dimensional electron gases

Focusing on the case of Rashba spin-orbit interaction, we then use this theory to extract the Rashba spin-orbit strength from weak antilocalization measurements in epitaxially grown InSb nanowires. We find a spin-orbit energy on the order of 0.25-1 meV.

TT 102.2 Thu 15:15 A 053

Tunable weak anti-localization in InAs nanowire device — •Libin Wang[1], Jingkun Guo[1], Sen Li[1], Ning Kang[1], Dong Pan[2], Jianhua Zhao[2], and Hongqi Xu[1] — [1]Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing 100871, China — [2]Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, China

III-V semiconductor nanowire had attracted much attention as a possible building block for future electronic systems because of its high performance and possibility of gate voltage manipulation of electron spins. InAs nanowires are particularly attractive due to its strong spin-orbit interaction. We report the fabrication and magnetotransport measurement of individual InAs nanowires with diameter of 40 nm on a SiO_2/Si substrate with a globe back gate. The observed magnetoresistance at low temperature can be used to estimate the characteristic phase coherence length and the spin-orbit scattering length. We observe a crossover between weak anti-localization and weak localization with the change of temperature and applied electric field. Our results give information on the fundamental spin relaxation and quantum coherence effect of InAs nanowire.

TT 102.3 Thu 15:30 A 053

Full-counting statistics of Landau-Zener interference in quantum dot arrays — •Michael Niklas[1], Robert Hussein[2], and Sigmund Kohler[2] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain

We investigate current cumulants for the transport in coupled quantum dots driven by a time-periodic field that sweeps the system repeatedly

through an avoided crossing and, thus, acts like a beam splitter. Consequently, as a function of the detuning and the driving amplitude, the cumulants exhibit Landau-Zener-Stückelberg-Majorana (LZSM) interference patterns similar to those observed for the current in driven double quantum dots [1]. These patterns indicate regions with sub- and super-Poissonian noise level. As a flexible method that allows us to study driving fields with arbitrary shape, we developed a propagation scheme for the iterative computation of current cumulants. We demonstrate that it is applicable also for larger systems such as quantum dot arrays or dimer chains.

[1] F. Forster et al., Phys. Rev. Lett. **112**, 116803 (2014).

TT 102.4 Thu 15:45 A 053

Fractionalized double quantum wires — •Tobias Meng[1,2] and Eran Sela[3] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [3]Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Tel Aviv, 69978, Israel

We discuss how electron-electron interactions can lead to novel phenomena in double quantum wire systems. Explicitly, we find that double wires with time reversal symmetry and strong electron-electron interactions can exhibit fractional conductances and cross-conductances in their normal state. They also allow to pump the fraction of a spin in their superconducting state. These effects are an extension of fractional helical Luttinger liquid physics, and can be understood as the one-dimensional cousins of bilayer fractional quantum Hall effects.

TT 102.5 Thu 16:00 A 053

Non-equilibrium Renormalization Group for Kondo Qdots in a Microwave Photon Field — •Andisheh Khedri[1,2,3], Ammar Nejati[1], and Johann Kroha[1] — [1]Universität Bonn — [2]RWTH Aachen — [3]FZ Jülich

Recent experiments on Kondo quantum dots in a static magnetic field and a microwave photon field show a resonant enhancement of the zero-bias differential conductance at a photon energy which scales with the applied magnetic field, but which is substantially larger than the bare Zeeman energy of the dot levels [1]. This behavior cannot be explained by direct, photoinduced spin-flip excitations of the dot. It points to a strong renormalization of the Zeeman energy (Landé factor) in the presence of the microwave field. We propose that the observed resonant conductance is caused by photo-assisted Kondo spin-flip scattering of the lead electrons, i.e., by electronic lead–dot transitions, assisted by coherent photon absorption and/or emission. We develop the non-equilibrium perturbative renormalization group (RG) theory [2] for this problem. The renormalization of the various coupling functions for spin vertices without photon processes as well as involving photon absorption, emission and scattering is anaylzed as well as the Qdot level shifts. We find a subtle interplay between Kondo scattering and coherent photoassisted processes, restoring the logarithmic RG flow and leading to strong renormalization of the Landé factor.

[1] B. Hemingway, S. Herbert, M. Melloch, A. Kogan, PRB **90**, 125151 (2014)
[2] A. Rosch, J. Paaske, J. Kroha, P. Wölfle, PRL **90**, 076804 (2003).

TT 102.6 Thu 16:15 A 053

Competing energy scales in the renormalization group flow of quantum dot setups with periodically varying parameters — •Katharina Eissing[1,2], Dante Marvin Kennes[1,2], and Volker Meden[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, 52074 Aachen, Germany — [2]JARA Fundamentals of Future Information Technology, 52056 Aachen, Germany

The functional renormalization group (fRG) has proven to be a versatile tool to investigate correlated, low-dimensional systems in and out of equilibrium. It was recently extended to study quantum dot setups with explicitly time dependent Hamiltonians [Phys. Rev. B 85, 085113 (2012)]. In systems in which one or more of the dot or lead parameters are varied periodically in time a periodic steady state is reached after all transients have died out. However, due to the limited simulation time the physics of this state can only be described, if we take advantage of the periodicity by combining the Floquet theorem and set up a functional RG with Green functions written in the Floquet basis. For the interacting resonant level model which in equilibrium and if driven by a time constant bias voltage is characterized by power-law scaling of observables in the relevant energy scales (e.g. temperature T or bias voltage V_b, respectively) with interaction dependent exponents this allows to investigate if and how the driving frequency Ω acts as a cutoff of the underlying renormalization group flow. The competition of this scale with the emergent low-energy scale T_K (Kondo scale) is investigated. I discuss how this competition is reflected in the observables characterizing the stationary transport through the dot.

15 min. break.

Invited Talk TT 102.7 Thu 16:45 A 053

Microscopic Origin of the 0.7-Anomaly in Quantum Point Contacts: Correlations in 1D — Florin Bauer[1], Jan Heyder[1], Dawid Borowsky[1], D. Taubert[1], D. Schuh[2], B. Bruognolo[1], Werner Wegscheider[3], Jan von Delft[1], and •Stefan Ludwig[1] — [1]Fakultät für Physik, LMU München — [2]Institut für Angew. Physik, Universität Regensburg — [3]ETH Zurich, Switzerland

Quantum point contacts (QPCs), the ultimate building blocks of quantum electronic circuits, are 1D constrictions in a 2D electron system (2DES). When a QPC is pinched off, its conductance famously decreases in integer steps of the conductance quantum, $G_Q = 2e^2/h$. An unexpected kink of the pinch-off curve near $0.7G_Q$ with an intriguing dependence on temperature, magnetic field and source-drain voltage, the 0.7-anomaly, has been subject of debates for the last two decades [1]. In this talk I will show that the divergence of the 1D density of states (DOS) at low energies, a prerequisite of the quantized conductance, is also the origin of the 0.7-anomaly. It naturally arises from strong correlations fostered by an enhanced DOS. They cause an anomalous increase of the spin susceptibility and back-scattering. Our microscopic model is built on a combination of systematic measurements of a highly tunable QPC and detailed numerical calculations [2]. We discuss commonalities and differences to previous more phenomenological attempts to explain the 0.7-anomaly, namely the model of spontaneous spin polarization and the Kondo model [1].

[1] A. Micolich, J. Phys.: Condens. Matter **23**, 443201 (2011)
[2] F. Bauer et al., Nature **501**, 73 (2013)

TT 102.8 Thu 17:15 A 053

Spin dynamics in a quantum point contact showing the 0.7-anomaly — •Dennis Schimmel[1,2], Florian Bauer[1,2], Jan Heyder[1,2], and Jan von Delft[1,2] — [1]Ludwig-Maximilians-Universitaet Muenchen — [2]Arnold Sommerfeld Center for Theoretical Physics

The 0.7-anomaly in the first conductance step of a quantum point contact is believed to arise from an interplay of geometry, spin dynamics and interaction effects. Various scenarios have been proposed to explain it, each evoking a different concept, including spontaneous spin polarization, or a quasi-localized state, or ferromagnetic spin fluctuations, or a van Hove ridge (a geometry-induced maximum in the density of states). Though these scenarios differ substantially regarding numerous details, they all imply anomalous dynamics for the spins in the vicinity of the QPC. Our model consists of a one-dimensional system with a parabolic barrier. Interactions are restricted to a central region around the barrier and short-range. The leads are solved exactly and the central region is then treated using the functional renormalization group within a coupled ladder approximation scheme. Within this setup, we have performed a detailed study of the spin dynamics in the central region by calculating the dynamical spin-spin correlation function $\chi(x,x',\omega) = \int_0^\infty \langle S_z(x,t)S_z(x',0)\rangle e^{i\omega t}$. We will discuss its behavior as function of frequency, interaction strength and gate voltage and comment on the implications of these results for each of the above-mentioned scenarios.

TT 102.9 Thu 17:30 A 053

Nonequilibrium transport through Anderson impurities: A comparative study based on continuous-time quantum Monte Carlo simulations and hierarchical quantum master equations — •Rainer Härtle[1], Guy Cohen[2], David R. Reichman[2], and Andrew J. Millis[3] — [1]Institut für theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Department of Chemistry, Columbia University, New York, USA — [3]Department of Physics, Columbia University, New York, USA

The hierarchical quantum master equation approach [1,2] is a promising new method for describing quantum impurity systems under nonequilibrium conditions. It employs a hybridization expansion with an advanced truncation scheme [2] to determine the time evolution of the impurity's density matrix from a product initial state. The method is a systematic expansion for which convergence can be demonstrated

so that numerically exact results can in principle be obtained. To elucidate the rigor of this procedure, we study the nonequilibrium dynamics of an Anderson impurity and benchmark the results with respect to continuous time quantum Monte Carlo methods [3]. The comparison shows excellent agreement as long as the temperature is above the Kondo scale. A discussion of the computational burden and of the scaling of numerical errors with truncation level is given. New results are presented for long-time dynamics arising in the presence of a magnetic field and/or an asymmetric coupling to leads.

[1] J. Jin et al., JCP 128, 234703 (2008).
[2] R. Härtle et al., PRB 88, 235426 (2013).
[3] G. Cohen et al., PRB 87, 195108 (2013).

TT 102.10 Thu 17:45 A 053

From thermal equilibrium to nonequilibrium quench dynamics: A conserving approximation for the interacting resonant-level — •Yuval Vinkler-Aviv[1,3], Avraham Schiller[3], and Frithjof B. Anders[2] — [1]Dahlem Center for Complex Quantum Systems and Fachberiech Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany — [3]Racah Institute of Physics, The Hebrew University, Jerusalem 91904, Israel

We develop a low-order conserving approximation for the interacting resonant-level model (IRLM), and apply it to (i) thermal equilibrium, (ii) nonequilibrium steady state, and (iii) nonequilibrium quench dynamics. The thermal equilibrium is used to carefully gauge the quality of the approximation by comparing the results with established methods such as renormalisation group approaches and establishes a good agreement for small interaction strengths. A closed expression for the nonequilibrium steady-state current is derived and analytically and numerically evaluated. We find a negative differential conductance at large voltages, and the exponent of the power-law suppression of the steady-state current is calculated analytically at zero-temperature. The response of the system to quenches is investigated for a single-lead as well as for two-lead setup at finite voltage bias, and results are presented for the time-dependent current for different bias and contact interaction strength.

[1] Phys. Rev. B **90**, 155110 (2014).

TT 102.11 Thu 18:00 A 053

Bound states in the continuum: Chiral lattices and van Hove singularities — •Jordi Mur-Petit and Rafael A. Molina — Inst. Estructura de la Materia, IEM-CSIC, Madrid, Spain

We present two distinct mechanisms for the formation of bound states in the continuum in lattices with van Hove singularities and/or chiral symmetry connected to leads. Bound states in the continuum (BICs) are square-integrable solutions of the time-independent Schrödinger equation with eigenenergies above the potential threshold. We derive some algebraic rules for the number of such states depending on the dimensionality and rank of the system Hamiltonian including the coupling to the leads. Next, we study the transport properties of relevant physical examples in square, honeycomb and triangular lattices, and propose different experiments to probe the presence of these BICs and related Fano resonances. Our results should find applications in a variety of set-ups, from semiconductor nanostructures to microwave resonator arrays, to cold atoms in optical lattices.

[1] V. Fernández-Hurtado, J. Mur-Petit, J.J. García-Ripoll, and R.A. Molina, New J. Phys. 16, 035005 (2014).
[2] J. Mur-Petit and R.A. Molina: Phys. Rev. B 90, 035434 (2014).

TT 102.12 Thu 18:15 A 053

Charge fluctuation effects in superconductor-quantum dot hybrid systems — •Sebastian Pfaller, Andrea Donarini, and Milena Grifoni — Institut I - Theoretische Physik Universität Regensburg

In a recent experiment [1] quasi particle transport through a carbon nanotube quantum dot coupled to superconducting (SC) leads was investigated both experimentally and theoretically. While most of the features could be explained by a perturbative theory up to lowest order in quasi particles tunnelling, other features like the broadening of the differential conductance peaks were not captured.

In order to account for these effects, we include charge fluctuation processes of quasi particles by extending the dressed second order theory of Kern *et al.* [2] to the case of SC leads. This yields an intrinsic broadening of the quantum dots energy levels, and, consequently, a renormalization of the sharp peaks coming from the BCS density of states. Moreover, new transport channels are obtained. They appear as peaks at zero and finite bias in the dI/dV-stability diagrams.

[1] M. Gaass, S. Pfaller, T. Geiger *et al.*, Phys. Rev. B **89**, 241405 (2014).
[2] J. Kern, and M. Grifoni, Eur. Phys. J. B **86**, 384 (2013).

TT 103: Transport: Poster Session

Time: Thursday 15:00–18:00 Location: Poster B

TT 103.1 Thu 15:00 Poster B

Currents in a chain of quantum dots — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP)Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Using the quantum kinetic equation analytical expressions for the currents in chains of quantum dots are derived. During the transient behaviour non-dissipative quantum correlations lead to a decay of the initial correlations. After this short time behaviour the total current for homogeneous electric fields is ballistic. For wavelength-modulated electric fields, effective capacitance, inductance and Ohmic resistance can be produced.

TT 103.2 Thu 15:00 Poster B

Phonon-induced spintronics and spin cooling in quantum dots — •Stephan Weiss[1], Jochen Brueggemann[2], Peter Nalbach[2], and Michael Thorwart[2] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [2]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg

In the presence of spin dependent tunnel couplings, vibrations in quantum dots or single molecule transistors induce exchange fields which give rise to spin-accumulation and -precession for confined electrons. The effective exchange field is calculated to lowest order in the dot-lead coupling for a nonequilibrium transport setup. For realistic parameters, an effective spin-phonon coupling driven by many-body interactions, either electron-phonon or Coulomb-like, emerges [1]. We investigate the precession- and accumulation-effects of the confined spins as function of bias- and gate-voltages. In addition, we investigate the cooling of a vibrational mode of a magnetic quantum dot by a spin-polarized tunneling charge current, exploiting the interaction between the magnetization and the vibration[2]. We determine parameter regimes for the *cooling* of the vibration below the lead temperature.

[1] S. Weiss, J. Brueggemann, and M. Thorwart, (submitted).
[2] J. Brueggemann, S. Weiss, P. Nalbach, and M. Thorwart, Phys. Rev. Lett. **113**, 076602 (2014).

TT 103.3 Thu 15:00 Poster B

Lab::Measurement — Measurement control and automation with Perl — Christian Butschkow, Alexei Iankilevitch, Alois Dirnaichner, Stefan Geissler, and •Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

For quickly setting up varying and evolving complex measurement tasks involving diverse hardware, graphical logic programming quickly reaches practical limits. We present *Lab::Measurement*, a collection of Perl modules designed to control instruments connected by as various means as GPIB, USB, serial cable, Oxford Instruments IsoBus, or Ethernet. Internally, backends as e.g. Linux-GPIB or National Instruments' NI-VISA library are used as well as direct operating system calls. Dedicated instrument driver classes relieve the user from taking care of internal details. An additional layer, Lab::XPRESS, enables fast and flexible creation of nested measurement loops, where e.g. several input variables are varied and one or several output parameters

are read for each setting. Metadata and device parameters are automatically protocolled. *Lab::Measurement* has already been successfully used in several low temperature transport spectroscopy setups. It is free software and available at `http://www.labmeasurement.de/`

TT 103.4 Thu 15:00 Poster B

Monitoring quantum transport: Backaction and measurement correlations — •Robert Hussein, Jorge Gómez-García, and Sigmund Kohler — Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, 28049 Madrid, Spain

We investigate a tunnel contact that is capacitively coupled to a double quantum dot and employed as charge monitor for the latter. We consider both the quantum regime and the classical limit characterized by the absence of quantum coherence. In the classical case, we derive measurement correlations from conditional probabilities, which yields quantitative statements about the parameter regime in which the detection scheme works well. Moreover, we demonstrate that not only the occupations of the double quantum dot may exhibit strong correlations with the detector current but also the corresponding current. The quantum mechanical solution shows that the backaction of the measurement tends to localize the electrons on the double quantum dot and, thus, significantly reduces the corresponding current. Furthermore, it provides the effective parameters of the classical treatment. It turns out that already the classical description is adequate for most operating regimes.

[1] R. Hussein, J. Gómez-García, and S. Kohler, Phys. Rev. B 90, 155424 (2014).

TT 103.5 Thu 15:00 Poster B

Long-range transfer of spin qubits — •Rafael Sánchez[1], Ghislain Granger[2], Louis Gaudreau[2], Fernando Gallego-Marcos[1], Michel Pioro-Ladrière[3], Sergei A. Studenikin[2], Andrew S. Sachrajda[2], and Gloria Platero[1] — [1]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain — [2]NRC, Ottawa, Canada — [3]Université de Sherbrooke, Canada

Quantum mechanics allows for superpositions of indirectly coupled states even if the intermediate states are far in energy. In transport, this enables long-range charge transfer through quantum dot chains [1,2]. We present the first evidence of long-range transfer of a spin qubit in a triple quantum dot [3]. This process is detected via a very narrow resonance in the current through the system at the degeneracy point of three-electron charge configurations (2,0,1) and (1,0,2). There, an electron is delocalized between the two dots without ever occupying the center dot. Of the two electrons forming a spin singlet in one dot, only the one with a spin opposite to that of the electron in the other edge dot will be allowed to tunnel. The emptiness of the centre dot warranties the conservation of the spin of the tunneling electron. Thus, the long-range electron tunneling between edges enables the long-range transfer of an arbitrary spin state (the qubit) in the opposite direction.

[1] M. Busl et al., Nature Nanotech. 8, 261 (2013).
[2] R. Sánchez et al., Phys. Rev. B 89, 161402(R) (2014).
[3] R. Sánchez et al., Phys. Rev. Lett. 112, 176803 (2014)

TT 103.6 Thu 15:00 Poster B

Conductance hysteresis during forming and breaking of single-atom contacts on Pb(111) — •Martin Müller[1], Nicolas Néel[1], Carlos Salgado[2], Juan Jose Palacios[2], and Jörg Kröger[1] — [1]Institut für Physik, TU Ilmenau, D-98693 Ilmenau — [2]Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain

Single-atom junctions were fabricated from Pb-coated W tips of a scanning tunneling microscope and a Pb(111) surface. Conductance traces were simultaneously recorded with tip approach up to contact and retraction. A pronounced hysteresis was observed between the abrupt formation of the contact and its gradual breaking. The hysteresis width and the conductance in contact depend on the tip geometry and contact position. Supporting ab initio calculations reproduce contact conductances and hysteresis widths and highlight the importance of the junction geometry. Financial support by the Carl Zeiss foundation is acknowledged.

TT 103.7 Thu 15:00 Poster B

Charge and Energy Transport through Quantum Dots — •Christian Schiegg, Michael Dzierzawa, and Ulrich Eckern — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

We consider a model of interacting spinless fermions coupled to non-interacting leads. Initially a non-equilibrium situation is imposed by applying a bias voltage and temperature gradient across the system. The time-evolution of the density matrix leads to a quasi-stationary state from which charge and energy currents can be extracted. Numerical results based on the time-dependent Hartree-Fock approximation are compared with exact currents obtained from discrete Hubbard-Stratonovich decoupling of the interaction for small systems. For a wide range of parameters the time-evolution of the currents is reasonably well described within the Hartree-Fock approach.

TT 103.8 Thu 15:00 Poster B

Scattering of two-dimensional Dirac fermions on gate-defined oscillating quantum dots — •Christian Schulz, Rafael L. Heinisch, and Holger Fehske — Universität Greifswald, Greifswald, Deutschland

Within an effective Dirac-Weyl theory we solve the scattering problem for massless chiral fermions impinging on a cylindrical time-dependent potential barrier. The set-up we consider can be used to model the electron propagation in a monolayer of graphene with harmonically driven quantum dots. For static small-sized quantum dots scattering resonances enable particle confinement and interference effects may switch forward scattering on and off. In addition to these phenomena, an oscillating quantum dot may cause the excitation of partial waves belonging to high energy states. This essentially modifies the resonance structures. For example, the scattering efficiency of an around the Dirac energy symmetric oscillating dot remains finite in the limit of low particle energies and small potential amplitudes. For an asymmetric oscillating dot, the partial wave resonances at higher energies are smeared out for small frequencies or large oscillation amplitudes, thereby dissolving the dot-bound states.

TT 103.9 Thu 15:00 Poster B

DC transport measurements of aluminium-oxide nanowire arrays — •Marco Pfirrmann[1], Sebastian T. Skacel[1], Jan N. Voss[1], Julian Münzberg[1], Martin Weides[1,2], Hannes Rotzinger[1], Hans E. Mooij[1,3], and Alexey V. Ustinov[1,4] — [1]Physikalisches Institut, Kalsruhe Institut of Technology, Wolgang-Gaede-Straße 1, D-76131 Karlsruhe, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, Staudinger Weg 7 D-55128 Mainz, Germany — [3]Kavli Institute of Nanoscience, Delft University of Technology, 2628 CJ Delft, The Netherlands — [4]Russian Quantum Center, 100 Novaya St., Skolkovo, Moscow region, 143025, Russia

We experimentally investigate superconducting aluminium-oxide nanowires with a focus on coherent quantum phase slips. In duality to the Josephson effect where two superconductors are weakly coupled through the tunneling of Cooper pairs, the tunneling of the phase across a nanowire leads to the quantum phase slip effect. We are interested in the DC transport properties of arrays of aluminium-oxide nanowires, where we expect to see spurs of quantum vortex dynamics in the *I-V* characteristics in dependence on the applied magnetic field. The high-resistive aluminium-oxide thin films are deposited by precise control of a reactive Al sputter plasma in oxygen atmosphere. Electron-beam lithography and reactive ion etching is used to define the nanowires. We present fabrication details and first measurement results of the parallel arrays of nanowires at mK temperatures.

TT 103.10 Thu 15:00 Poster B

Light-induced changes of the electronic transport of atomic-sized contacts — •Matthias Bädicker, Daniel Benner, Golaleh Ghafoori, Johannes Boneberg, and Elke Scheer — Universität Konstanz, Germany

We investigate the influence of laser light onto the electrical transport of atomic sized Au contacts realized by the mechanically controllable break junction (MCBJ) technique. Experiments on MCBJs showed light-induced conductance changes, which have been interpreted as photo-assisted transport due to the excitation of high-energetic quasiparticles and collective effects such as surface plasmon excitation. Also optical near field enhancement caused by antenna effects as well as thermal expansion and thermo power may contribute to the signal [1-4]. The influence of surface plasmons is of particular interest for this work, because they provide a way to bring light to the contact without illuminating it directly. To excite and detect surface plasmons we fabricated grating couplers at either side of the constriction. Optical measurements carried out simultaneously with the transport measure-

ments confirm the excitation and transmission of surface plasmons through the constriction [5,6]. In this work we concentrate on time-resolved transport experiments to distinguish between heating effects [7] and influences due to the electric field modulation of the plasmons.

[1] J.K. Viljas et al., PRB 75, 075406(2007).
[2] D. Guhr et al., PRL 99, 086801 (2007).
[3] N. Ittah et al., Nano Lett. 11, 2 (2011).
[4] Nano Lett. 9, 4 (2009).
[5] D. Benner et al., New J. Phys. 15 113014.
[6] Nano Lett., 14(9) (2014).
[7] A. Ganser et al., APL 105, 191119 (2014).

TT 103.11 Thu 15:00 Poster B

Probing Molecular Transport by Multiple Andreev Reflections — •David Weber and Elke Scheer — Universität Konstanz, Konstanz, Germany

The properties of molecular transport can be analyzed by measuring the conductance G or its derivatives, giving first insights to molecular levels and coupling to the electrodes [1]. Yet, the information of the intrinsic composition of conduction channels in a molecular contact is very limited. A Pt-H_2-Pt junction with a conductance of 1 G_0 was shown to accommodate indeed a single perfectly transmitted channel by measurements of the shot noise [2]. For Au-1,4-Benzenedithiol-Au junctions it has been proposed that despite of an enormous variability of G from 0.001 G_0 to almost 1 G_0, the transport would be maintained by a single channel [3]. We test this proposition by coupling the junction to superconducting leads and analyzing the non-linear current-voltage characteristics [4]. We present first results obtained with a low temperature Mechanically Controlled Break Junction setup.

[1] L. Zotti et al., Small **6**, 1529-1535 (2010)
[2] R. H. M. Smit et al., Nature **419**, 906-909 (2002)
[3] Y. Kim et al., Nano Lett. **11**, 3734-3738 (2011)
[4] J. C. Cuevas et al., Phys. Rev. B **54**, 7366-7379 (1996)

TT 103.12 Thu 15:00 Poster B

Transport Calculations for Si_4 Clusters with Gold single Atom Contacts — •Jeffrey Kelling[1], Jochen Kerbusch[1,2], Artur Erbe[1], Rainer Dietsche[3], Gerd Ganteför[3], Elke Scheer[3], Peter Zahn[1], and Sibylle Gemming[1,4] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Center for Advancing Electronics Dresden (CFAED), Technische Universität Dresden, Dresden, Germany — [3]Physics Department, University of Konstanz, Konstanz, Germany — [4]Institute of Physics, TU Chemnitz, Chemnitz, Germany

We present results for electronic transport through Si_4 clusters contacted by single-atom gold contacts attached to <111> fcc-gold leads. The calculations were performed using density functional theory and the non-equilibrium Green's function approach for transport. The simulation setup mimics contacts in mechanically controllable break-junction experiments, which provide data for comparison.

TT 103.13 Thu 15:00 Poster B

Enhanced thermoelectric figure of merit in polycrystalline carbon nanostructures — •Thomas Lehmann[1,2,3], Dmitry Ryndyk[1,2,3], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCCMS), TU Dresden, 01062 Dresden, Germany — [3]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany

Grain boundaries are commonly observed in carbon nanostructures, but their influence on thermal and electronic properties are still not completely understood. Using a combined approach of density functional tight-binding theory and non-equilibrium Green functions we investigate electron and phonon transport in carbon based systems. In this work, quantum transport and thermoelectric properties are summarized for graphene sheets, graphene nanoribbons and carbon nanotubes with a variety of grain boundary types in a large temperature range. Motivated by previous findings that disorder scatters phonons more effectively than electrons, a significant improvement in the thermoelectric performance for polycrystalline systems is expected. While the effect depends on the grain boundary type, we demonstrate that grain boundaries are a viable tool to greatly enhance the thermoelectric figure of merit, paving the way for the design of new thermoelectric materials.

TT 103.14 Thu 15:00 Poster B

Electron transport in Diarylethene Switches: A combined theoretical and experimental approach — •Lokamani Lokamani[1], Torsten Sendler[1], Peter Zahn[1], Sibylle Gemming[1,2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf e.V., Germany — [2]SKALMOD, Institute of Physics, TU-Chemnitz, Germany

Diarylethene, a class of photosensitive molecules which exhibit photochoromism, can be switched optically between open- and closed-ring isomers. The open-ring isomer is non-planar with the pi-system localized on two aryl groups. On the other hand, the closed-ring isomer is highly planar with the pi-conjugated-system extending over the whole molecule. In break-junction experiments diarylethene in open and closed-ring isomeric form can be distinguished by a low or high conductance state with a difference in current levels of about an order of magnitude. Moreover, these molecules exhibit stable current-voltage characteristics in both the conductance states.

Here, we study the electronic transport properties of such derivatives at the level of single molecules using density functional theory and non-equilibrium greens function. In particular, we analyse the effect of strongly electrophillic groups on conductance properties of single molecules attached to gold electrodes. A comparison to break junction experimental results is also presented.

TT 103.15 Thu 15:00 Poster B

Switching a Molecular Junction using a Proton Transfer Reaction — •Chriszandro Hofmeister, Pedro B. Coto, and Michael Thoss — Institut für Theoretische Physik und Interdisziplinäres Zentrum für Molekulare Materialien (ICMM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

The possibility of utilizing single molecules as switches in electronic circuits has motivated intensive experimental and theoretical research on bistable molecular systems [1]. In this contribution, we present a theoretical model for the switching of a molecular junction based on a ground state proton transfer reaction triggered by an external electrostatic field [2,3]. The dynamics of the proton translocation and the electron transport across the junction is described within the framework of quantum master equations. The results show that the proton transfer induces a significant change in the current for low bias voltages. The underlying mechanisms are analyzed in some detail.

[1] S.J. van der Molen *et al.*,
J. Phys.: Condens. Matter 22, 133001 (2010)
[2] A.L. Sobolewski, Phys. Chem. Chem. Phys. 10, 1243 (2008)
[3] C. Hofmeister *et al.*, J. Mol. Model. 20, 1 (2014)

TT 103.16 Thu 15:00 Poster B

Magneto resistance measurements on ultra clean CNT devices with ferromagnetic contacts — •Michael Schafberger, Nicola Paradiso, Michael Görtler, Helmut Körner, Tobias Weindler, Matthias Kronseder, Andreas K. Hüttel, and Christoph Strunk — Institute of Exp. and Appl. Physics, University of Regensburg, Germany

Our goal is the realization of a spin-valve device based on ultra-clean single wall carbon nanotubes (SWNTs). In order to grant defect free and unperturbed SWNTs , chemical vapor deposition (CVD) growth is performed as last nanofabrication step. The achievement of ferromagnetic contacts that can sustain the CVD conditions remains to date elusive. We investigate bilayers of Rhenium and Cobalt (20/40 nm), which form an alloy during the CVD. The Re/Co contacts have been characterized by vibrating sample and SQUID magnetometry in order to demonstrate the persistence of ferromagnetic behavior after CVD. Optimized devices have then been used for transport measurements in the Coulomb blockade regime at 20 mK. The results of magnetoresistance experiments will be discussed together with recently proposed alternative fabrication approaches.

TT 103.17 Thu 15:00 Poster B

Effect of geometrical Langevin forces on magnetic dynamics — •Tim Ludwig[1] and Alexander Shnirman[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]DFG-Center for Functional Nanostructures (CFN), Karlsruher Institut für Technologie, Karlsruhe, Germany

Stochastic Landau-Lifshitz-Gilbert (LLG) equations with Langevin forces are a standard tool to describe the magnetic dynamics of fer-

romagnetic single-domain particles. In the classical regime, i.e. for temperatures much higher than the precession frequency, the results of Brown [1] can be used. Recently, it was predicted that, at low temperatures, the Langevin forces are influenced by the geometrical phases [2]. We analyzed the LLG-type Langevin equations with the geometrical Langevin forces for the situation of ferromagnetic resonance. At low temperatures, we found that the stationary distribution of the magnetization is governed by an effective geometric temperature rather than by the bath temperature.

[1] W. F. Brown, Phys. Rev. **130**, 1677 (1963).
[2] A. Shnirman, Y. Gefen, A. Saha, I. S. Burmistrov, M. N. Kiselev, and A. Altland, arXiv:1409.0150v1.

TT 103.18 Thu 15:00 Poster B

Emerging Magnetism in transition metal atomic contacts — •Martin Keller[1], Amin Karimi[1], Florian Strigl[1], Bernat Olivera[2], Carlos Untiedt[2], Elke Scheer[1], and Torsten Pietsch[1] — [1]Department of Physics, University of Konstanz, 78467 Konstanz, Germany — [2]Department of Applied Physics, University of Alicante, 03690 Alicante, Spain

Transition metals which are a strong paramagnet (Pd, Pt) or have only weak magnetic order (Gd) show fascinating magnetic properties in reduced dimensions. For Pd nanowires anisotropic magnetotransport magnetic effects are theoretically predicted [1,2], while, as we show, Gd exhibits large magnetostriction in atomic contacts. These properties can be examined by investigating the magnetoconductance (MC) of controlled atomic-size junctions of these materials. Additional a study of the shot noise of such atomic junctions provides information that cannot be easily obtained by other means, such as the determination of the transmission probability and the number of electronic conductance channels [3]. Here we show a comprehensive experimental study of MC and shot noise of atomic contacts of these metals. We also develop a minimal model for magnetic configuration of the contatcs to account for the complex MC behavior.

[1] Delin et al., Phys. Rev. Lett. 92, 057201 (2004).
[2] Smelova et al., Phys. Rev. B. 77, 033408 (2008).
[3] Brom et al., Phys. Rev. Lett. 82, 1526 (1999).

TT 103.19 Thu 15:00 Poster B

Coherent Dynamics of Quantum Spins in Magnetic Environments — •Lars-Hendrik Frahm, Christoph Hübner, Benjamin Baxevanis und Daniela Pfannkuche — 1. Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany

We investigate equilibration and transport effects of a quantum spin that is exchange coupled to two electron reservoirs. We include an effective crystal field, which arises from the substrate the spin is living on and gives the spin an easy axis for alignment. First, we determine stationary states using a quantum master equation and compare our results to a semi-classical approach using a rate equation. Second, we consider a spin-polarized electron reservoir that breaks the rotation symmetry around the spin quantization axis. This system requires to consider the complete density operator, where its knowledge allows to calculate magnetization dynamics and transport properties on an equal footing. We discuss the electron transport through the spin system by especially focusing on the non-linear influence of the spin torque effect.

TT 103.20 Thu 15:00 Poster B

Nanomechanics and strain engineering in 2d materials — •Alexander Croy[1], Daniel Midtvedt[1], and Caio H. Lewenkopf[2] — [1]Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany — [2]Universidade Federal Fluminense, Niterói, Brazil

We investigate the electromechanical coupling in two-dimensional materials. To this end we put forward a systematic approach to relate the macroscopic strain tensor to microscopic atomic displacements. This strain-displacement relation depends non-trivially on the lattice structure and the parameters of the force field model. Implications for nanomechanical properties and electromechanical coupling in two-dimensional materials are discussed. Using graphene as a study case, we combine a tight binding and a valence force-field model to calculate the electronic (DOS, band energy) and mechanical properties (elastic modulus, Poisson ratio) of graphene nanoribbons under strain. We then compare those calculations with results obtained from the Dirac equation coupled to continuum mechanics. In this long wave-limit effective theory we find a renormalization correction to the strain-induced pseudo-magnetic fields which is connected to the strain-displacement relation.

TT 103.21 Thu 15:00 Poster B

Emulation of the Fermi-Hubbard Model in One Dimension — •Jan-Michael Reiner, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

For every qubit system which allows for σ_z and σ_x coupling between the qubits, it is possible to realize a Hamiltonian which is similar to the Fermi-Hubbard model in 1D. This way one can design a quantum emulator for this model.

We discuss a specific implementation of such an emulator for superconducting qubits. We consider tunable Transmon qubits, where the σ_z coupling is realized via inductive coupling and the σ_x coupling is realized via capacitive coupling. We then discuss the possible errors through disorder and how confidence in the emulation results can be established through measurements of local operators.

TT 103.22 Thu 15:00 Poster B

Towards a room temperature 2D quantum platform on diamond — •Nathan Chejanovsky[1,2] and Jörg Wrachtrup[1,2] — [1]3rd Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, 70174 Stuttgart, Germany

The nitrogen vacancy (NV) in diamond has been on the fore front of research for room temperature quantum computation applications. Polarization of nuclear spins using the NV center electron spin as a quantum bus for read/write has been demonstrated [1]. For material residing on top of the diamond lattice, a suitable platform is needed for nuclei spin polarization. It has been proposed that graphene, covalently bonded to other non-zero spin nuclei, could be a starting point for this platform [2]. However, graphene alone contains a zero band gap which quenches the NV- state, rendering it useless for optical read out.

We propose here a different approach using 2D hexagonal boron-nitride (h-BN) monolayer instead. These monolayers have shown a band gap from 4.6 to 7.0 eV [3]. In addition, all atoms composing the monolayer already have none zero spin: Boron*s isotope natural abundance is 80.1% spin 3/2 and 19.9% spin 3, for Nitrogen the abundance is 99.6% spin 1 and 0.4% spin 1/2. These properties make h-BN an excellent choice for a starting 'playground' platform for NV controlled quantum applications.

[1] Taminiau, T. H. et al. Nature Nanotechnology 9, 171-176 (2014)
[2] Cai, J. et al. Nature Physics 9, 168-173 (2013)
[3] Nagashima, A. et al. Physical Review B 51, 4606-4613 (1995).

TT 103.23 Thu 15:00 Poster B

Decoherence in Two-Level Systems — •Sebastian Zanker[1], Jürgen Lisenfeld[2], Michael Marthaler[1], Gerd Schön[1], Alexey Ustinov[2], and Georg Weiss[2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [2]Physikalisches Institut, Karlsruhe Institute of Technology , D-76131 Karlsruhe, Germany

We study decoherence of two level systems (TLS) living inside the amorphous AlOx layer of a phase qubit's Josephson junction. We discuss TLS coupling to phonons, tunneling quasiparticles and other TLS as possible sources of decoherence and compare theoretical decoherence behavior with experimental data. The experiment suggests strong improvements in dephasing times using spin echo protocol as compared to Ramsey dephasing, $\Gamma_{\mathrm{Ramsey}}/\Gamma_{\mathrm{echo}} \sim 3-55$ which indicates a divergent noise spectral density at low frequencies best matched by either other TLS or quasiparticles.

TT 103.24 Thu 15:00 Poster B

Nonequilibrium spin noise and noise of susceptibility — •Pablo Schad[1], Boris N. Narozhny[1,2], Gerd Schön[3,4], and Alexander Shnirman[1] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [2]National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe shosse 31, 115409 Moscow, Russia — [3]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [4]Institut für Nanotechnologie, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany

We analyze out-of-equilibrium fluctuations in a driven spin system and relate them to the noise of spin susceptibility. In the spirit of the linear

response theory we further relate the noise of susceptibility to a 4-spin correlation function in equilibrium. We show that, in contrast to the second noise (noise of noise), the noise of susceptibility is a direct measure of non-Gaussian fluctuations in the system. We develop a general framework for calculating the noise of susceptibility using the Majorana representation of spin-1/2 operators. We illustrate our approach by a simple example of noninteracting spins coupled to a dissipative (Ohmic) bath.

[1] P. Schad, B. N. Narozhny, G. Schön, and A. Shnirman, Phys. Rev. B 90, 205419 (2014).

TT 103.25 Thu 15:00 Poster B

Influence of strong noise on coupled qubit systems — •Philipp Rudo, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, KIT, Karlsruhe

We investigate the influence of the environment on systems with coupled qubits. For this we assume that the coupling between the qubits as well as the coupling of the qubit to its environment is strong. In our model we are especially interested in the choice of basis when the qubit undergo an adiabatic evolution while the noise is static. To do so we introduced an rotation angle connecting the different bases of the adiabatic evolution and investigate its behavior over time.

TT 103.26 Thu 15:00 Poster B

Transmon qubits coupled to lumped element LC-readout-resonators — •Joel Cramer[1], Peter Fehlner[1], Jochen Braumüller[1], Steffen Schlör[1], Lucas Radtke[1], Hannes Rotzinger[1], Martin Weides[2,1], and Alexey V. Ustinov[3,1] — [1]Physikalisches Institut, KIT, Wolfgang-Gaede-Straße 1, 76131 Karlsruhe, Germany — [2]Institut für Physik, JGU, Staudingerweg 7, 55128 Mainz, Germany — [3]Russian Quantum Center, 100 Novaya St., Skolkovo, Moscow, 143025, Russia

Superconducting qubits are among the most promising approaches for unit cells of a quantum computer or simulator. In this work, we investigated capacitively shunted Cooper pair boxes, so-called transmon qubits, each of them coupled to a superconducting readout resonator. Significant detuning of resonator and qubit enables non-demolition readout of the qubit state. Transmon qubits offer simple design and, in principle, large coherence time. In this work quasi-lumped element LC-resonators have been employed,which allow a compact qubit-resonator design of about $400 \times 600\,\mu\mathrm{m}^2$. In total one chip contains 12 qubit-resonator pairs, each linked to its own fast-flux bias line. To implement and test these circuits, we have chosen simple optical lithography of aluminum films deposited on sapphire substrates. This approach results in relatively large junction sizes and reduced lifetimes due to large number of parasitic two-levels states within the tunnel barrier. Time domain measurements of the fabricated system revealed T1 lifetime of about $0.5\,\mu$s, long enough to explore quantum phenomena like multi-level dressing.

TT 103.27 Thu 15:00 Poster B

Tunable Nb resonators for resonant coupling with ultracold atomic gases — •Benedikt Ferdinand, Daniel Bothner, Dominik Wiedmaier, Dieter Koelle, and Reinhold Kleiner — Physikalisches Institut and Center for Collective Quantum Phenomena in LISA$^+$, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany

We intend to investigate a hybrid quantum system where ultracold atomic gases play the role of a long-living quantum memory, coupled to a superconducting qubit via a transmission line resonator. As a first step towards this goal we develop a tunable superconducting resonator-chip containing a Z-shaped trapping wire for the atoms. Schemes for trapping the atoms in close vicinity of the resonator gap for maximum coupling are presented. We forthermore show how one can retain the full microwave performance despite these additional wire structures. For resonant coupling it is beneficial to have a tunable resonator which is insensitive to applied magnetic fields. Therefore we add a ferroelectric tunable capacitance with small dimensions compared to the resonator length. Experimental results of the controlled tunability are shown.

TT 103.28 Thu 15:00 Poster B

Circuit QED with 3D cavities — •Edwar Xie[1,2,3], Gustav Anderson[1,2], Lujun Wang[1,2], Alexander Baust[1,2,3], Peter Eder[1,2], Michael Fischer[1,2], Jan Goetz[1,2], Max Haeberlein[1,2], Manuel Schwarz[1,2], Karl Friedrich Wulschner[1,2], Ling Zhong[1,2,3], Frank Deppe[1,2], Kirill Fedorov[1,2], Hans Hübl[1,2], Achim Marx[1], Edwin Menzel[1,2], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

In typical circuit QED systems on-chip superconducting qubits are coupled to integrated coplanar microwave resonators. Due to the planar geometry, the resonators are often a limiting factor regarding the total coherence of the system. Alternatively, similar hybrid systems can be realized using 3D microwave cavities.

Here, we present design considerations for the 3D microwave cavity as well as the superconducting transmon qubit. Moreover, we show experimental data of a high purity aluminum cavity demonstrating quality factors above $1.4 \cdot 10^6$ at the single photon level and a temperature of 50 mK. Our experiments also demonstrate that the quality factor is less dependent on the power compared to planar resonator geometries. Furthermore, we present strategies for tuning both the cavity and the qubit individually.

This work is supported by the DFG via SFB 631 and the EU projects CCQED and PROMISCE.

TT 103.29 Thu 15:00 Poster B

Circuit QED with transmon qubits — •Karl Friedrich Wulschner[1,2,3], Javier Puertas[1,2,3], Alexander Baust[1,2,3], Peter Eder[1,2,3], Michael Fischer[1,2,3], Jan Goetz[1,2,3], Max Haeberlein[1,2,3], Manuel Schwarz[1,2,3], Edwar Xie[1,2,3], Ling Zhong[1,2,3], Frank Deppe[1,2,3], Kirill Fedorov[1,2,3], Hans Hübl[1,3], Achim Marx[1,2,3], Edwin Menzel[1,2,3], Martin Weides[4], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany — [4]Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Superconducting quantum bits are basic building blocks for circuit QED systems. Applications in the fields of quantum computation and quantum simulation require long coherence times. We have fabricated and characterized superconducting transmon qubits which are designed to operate at a high ratio of Josephson energy and charging energy. Due to their low sensitivity to charge noise transmon qubits show good coherence properties. We couple transmon qubits to coplanar waveguide resonators and coplanar slotline resonators and characterize the devices at mK-temperatures. From the experimental data we derive the qubit-resonator coupling strength, the qubit relaxation time and calibrate the photon number in the resonator via Stark shifts.

This work is supported by the DFG via SFB 631 and the EU projects CCQED and PROMISCE.

TT 103.30 Thu 15:00 Poster B

Implementation of a time domain measurement setup for circuit QED experiments — •Miriam Müting[1,2], Jan Goetz[1,2], Alexander Baust[1,2,3], Peter Eder[1,2], Michael Fischer[1,2], Max Haeberlein[1,2], Manuel Schwarz[1,2], Karl Friedrich Wulschner[1,2], Ling Zhong[1,2,3], Frank Deppe[1,2], Kirill Fedorov[1,2], Hans Hübl[1,2], Achim Marx[1], Edwin Menzel[1,2], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

For many experiments and applications of circuit QED systems the time evolution of the quantum system plays an important role. Therefore, studies of the quantum dynamics in the time domain are essential. Here, we present a time domain excitation and readout scheme, which allows us to investigate the quantum behavior of coupled qubit-resonator systems. We apply this scheme to perform Rabi and echo measurements to fully characterize our systems. Additionally, we investigate the decoherence properties at various operation points definded by the applied magnetic flux. Our readout scheme is promising for future simulation experiments of relativistic quantum systems.

This work is supported by the DFG via SFB 631 and the EU projects CCQED and PROMISCE.

TT 103.31 Thu 15:00 Poster B

The two classes of low energy spectra in finite carbon nanotubes — •Magdalena Marganska[1], Piotr Chudzinski[1,2], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, Regensburg

University, 93 053 Regensburg, Germany — [2]Institute for Theoretical Physics, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands

Electrons in carbon nanotubes (CNTs) possess spin and orbital degrees of freedom. The latter is inherited from the bipartite graphene lattice with two inequivalent Dirac points. The electronic spectra obtained in several transport experiments on CNT quantum dots in parallel magnetic field often show an anticrossing of spectral lines assigned to the opposite Dirac valleys. So far this valley mixing has been attributed to the disorder, with impurity induced scattering with large momentum transfer. We show that this effect can arise also in ultraclean armchair-like CNTs, where it is caused solely by the presence of the boundaries. In zigzag-like CNTs it does not occur due to the angular momentum conservation - there the two valleys indeed correspond to different values of orbital angular momentum. In the armchair-like CNTs the orbital angular momentum in both valleys is zero and the degeneracy between valley states is removed. The magnitude of the level splitting depends in a non-monotonous way on the energy of the levels involved.

TT 103.32 Thu 15:00 Poster B

Effect of Hydrogen on Spin-Transport in Graphene — •Fedor Tkatschenko, Jan Bundesmann, Denis Kochan, Jaroslav Fabian, and Klaus Richter — Institut für Theoretische Physik, Universität of Regensburg, 93053 Regensburg Germany

The impact of hydrogen on the spin lifetime is expected to be huge, as it leads to resonant scattering near the charge neutrality point [1] and to the formation of local magnetic moments in the vicinity of the hydrogen. This situation strongly enhances the spin flip probability of electrons and holes when passing through a graphene sample.

Here we aim to explain the experimental results [2], which seem to contradict the theoretical predictions, by taking into account the formation of hydrogen clusters, which reduce the effect on the spin lifetime compared to isolated hydrogen atoms. We calculate the electronic structure of hydrogenated graphene and perform quantum transport calculations based on a tight-binding model. Adopting the parameters from ab initio calculations, we find that clustering affects both, the formation of the resonant state and the magnetic moments. We show that the exact configuration, such as the sublattice occupation of each cluster is essential, as it decides for example if local magnetic moments are formed and determines the position of the resonant state.

[1] D. Kochan, M. Gmitra and J. Fabian PRL **112**, 116602 (2014)
[2] M. Wojtaszeck, I. J. Vera-Marun, T. Massen and B. J. van Wees PRB **87**, 081402(R) (2013)

TT 103.33 Thu 15:00 Poster B

Dirac Electrons in a Photon Cavity — •Lisa Hesse and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We consider low energy excitations of monolayer graphene embedded in an optical cavity and exposed to a perpendicular constant magnetic field. The influence of an additional radiation field can yield resonant cyclotron transitions of the Dirac fermions of graphene which can be studied using techniques known from cavity quantum electrodynamics. The coupling of cavity photons with condensed matter has been realized in the context of electron gases[1] and recently also proposed for graphene[2, 3] and therefore opens a new subfield of research in graphene. Based on a realistic tight-binding model, we consider the interaction of cavity photon modes with Landau quantized states in graphene and study the spectral properties of this hybrid system.

[1] G. Scalari, C. Maissen, D. Turčinková, D. Hagenmüller, S. De Liberato, C. Ciuti, C. Reichl, D. Schuh, W. Wegscheider, M. Beck, and J. Faist, Science 335, 1323 (2012).
[2] D. Hagenmüller and C. Ciuti, Phys. Rev. Lett. 109, 267403 (2012).
[3] L. Chirolli, M. Polini, V. Giovannetti and A. H. MacDonald, Phys. Rev. Lett. 109, 267404 (2012).

TT 103.34 Thu 15:00 Poster B

Charge transport through structurally well-defined graphene nanoribbons — •Nils Richter[1], Akimitsu Narita[2], Andrea Candini[3], Xinliang Feng[4], Klaus Müllen[2], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg Universität, Mainz, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany — [3]Centro S3, Istituto Nanoscienze CNR, Modena, Italy — [4]TU Dresden, Dresden, Germany

Graphene nanoribbons are ultra narrow stripes of graphene, a monolayer material of carbon atoms. Such ribbons are of particular interest because of the new physical phenomena that arise due to their geometrical confinement. Theory predicts a band gap that is dependent on width and edge structure of the ribbons [1]. In chemically synthesized graphene nanoribbons the edge structure is perfect on the atomic level [2]. For the investigation of the charge and spin transport properties we rely on fabricating contacts to the ribbons using the electromigration technique. Nanoribbons that are dispersed in a solvent can then be drop cast on top of these nanojunctions. Besides junctions formed in normal metals we explore graphitic electrodes [3] and ferromagnetic metal electrodes [4]. Using ribbons with different widths and edge geometries, we probe the exciting unconventional properties that have been predicted for these nano-structures [5].

[1] K. Nakada et al. Phys. Rev. B, 54, 24 (1996).
[2] A. Narita et al., Nature Chem. 6, 126 (2014).
[3] A. Candini et al., Beilstein Journal of Nanotechnology, submitted (2014).
[4] A. Bieren et al., Phys. Rev. Lett. 110, 067203 (2013).
[5] O. Yazyev, Rep. Prog. Phys. 73, 056501 (2010).

TT 103.35 Thu 15:00 Poster B

Transport measurements in graphite-like C_3B and C_3P — •Philip Brown[1], Timothy King[2], Peter Matthews[2], Dominic Wright[2], and Malte Grosche[1] — [1]Dept. of Physics, 19 J J Thomson Ave, Cambridge CB3 0HE, United Kingdom — [2]Dept. of Chemistry, Lensfield Road, Cambridge CB2 1EW, United Kingdom

Heavily-doped graphitic materials are of both fundamental and practical interest. Pure bulk graphite is a semimetal exhibiting unusual linear magnetoresistance at low temperatures, and the Dirac point in monolayer graphene leads to a plethora of interesting physics. The effects of boron doping have been investigated theoretically in some detail.

$C_{1-x}B_x$ is predicted to dramatically improve upon the already high Li ion storage of graphite, and may also have relevance as a functional material for fusion reactor cladding. The $x = 0.25$ compound C_3B has been synthesised experimentally, and found to possess graphite's hexagonal lattice and an ordered 2D structure. Despite extensive theoretical study, little experimental data is available on the properties of these heavily doped graphitic materials.

We report magnetotransport measurements on bulk samples of C_3B and C_3P, in temperatures down to 2 K and fields up to 9 T. We find both materials are semiconducting. The resistivity exhibits a non-Arrhenius temperature dependence over a wide range. At low temperatures, the dependence of resistivity on field is nearly linear and does not saturate in fields up to 9 T. Our findings are discussed in the context of current theoretical models of these novel materials.

TT 103.36 Thu 15:00 Poster B

Transport measurements on epitaxial $Bi_{1-x}Sb_x$ thin films grown on Si(111) — •Julian Koch, Philipp Kröger, Herbert Pfnür, and Christoph Tegenkamp — Leibniz Universität Hannover, Inst. für Festkörperphysik, Appelstr. 2, 30167 Hannover

The alloy $Bi_{1-x}Sb_x$ is a 3D topological insulator for concentrations between x = 0.04 and 0.22 [1]. Thus it has topologically protected metallic surface states and an insulating bulk at these concentrations, making it interesting for transport measurements. In this study thin films are used to reduce bulk contributions and to provide the possibility of nanostructuring. The films are grown by in-situ co-deposition on Si(111) substrates. The morphology has been controlled by means of low energy electron diffraction. Temperature dependent transport measurements for temperatures from 12 to 300 K were performed for films of different stoichiometry ranging from $x = 0.14 - 0.22$ and thicknesses of 10, 20, 40 and 60 BL. Besides variable range hopping and activated bulk transport, metallic surface transport channels have been identified. At 10 BL the surface transport is strongly suppressed in accordance with measurements on Bi_2Se_3 [2]. Furthermore, magnetotransport measurements up to 4 T were performed in order to determine carrier concentrations, mobilities and scattering times. A 30 BL film with a concentration of x = 0.18 was found to have carrier concentrations of $n = 1 \cdot 10^{13}$ cm^{-2} and $p = 2 \cdot 10^{13}$ cm^{-2} with mobilities of $\mu_n = 2.6 \cdot 10^2$ cm^2(Vs)$^{-1}$ and $\mu_p = 1.9 \cdot 10^2$ cm^2(Vs)$^{-1}$. Compared to Bi(111)-films the spin-orbit scattering rate is reduced by one order of magnitude.

[1] PRB **83**, 201104(R).
[2] PRL **109**, 066803

TT 103.37 Thu 15:00 Poster B

First investigations of the sputter deposited topologically non-trivial ternary Heusler YPdBi — •Robin Klett[1], Jan Krieft[1], Benedikt Ernst[2], Daniel Ebke[2], Claudia Felser[2], and Günter Reiss[1] — [1]CSMD, Physics Department, Bielefeld University, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

A large number of ternary Heusler compounds have been recently proposed as three-dimensional topological insulators with tunable physical properties. However, no transport measurements associated with the topological surface states have been observed in these candidates due to the dominating conduction contribution from bulk. In this work, we investigate the physical properties of sputter deposited topologically non-trivial half-Heusler non-centrosymmetric semimetal YPdBi thin films. First measurements indicate fingerprints of Weak Antilocalization effects and a superconducting phase transition at roughly 4K.

TT 103.38 Thu 15:00 Poster B

Pd/PtBi based topological insulators prepared by sputter deposition — •Benedikt Ernst[1], Daniel Ebke[1], Stanislav Chadov[1], Robin Klett[2], Günter Reiss[2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Thin Films and Physics of Nanostructures, Bielefeld University, Germany

Heusler compounds have exhibited manifold physical properties in the recent years and attracted a lot of interest in the field of spintronic applications due to their half-metallic properties.

In this work, we have prepared Heusler materials such as LaPdBi, LaPtBi and YPtBi for which a topological insulating behavior was predicted. In a combinatorial approach we used a mixture of Pd and Pt to tune the band gap. Co-deposition by DC- and RF magnetron sputtering was used to prepare corresponding thin films. To realize an epitaxial film growth in the crystallographic $C1_b$ structure on MgO-substrates, a buffer layer was applied and optimized. Initial transport properties will be discussed with regard to the film composition and the crystallographic properties.

TT 103.39 Thu 15:00 Poster B

High quality thin films of $BaBiO_3$ on $SrTiO_3$ grown by pulsed laser deposition — •Michael Zapf[1], Martin Stübinger[1], Gang Li[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — [2]Institut für Theoretische Physik und Astronomie, Universität Würzburg, Germany

Recently, $BaBiO_3$ (BBO) has been predicted to be a possible candidate for a large gap topological insulator. However, DFT calculations show that the protected surface states are located 2 eV above the Fermi level. To populate these states heavy electron doping is necessary. Conceivable ways to achieve such a doping are, for example, the deposition of alkali metal atoms on thin BBO films or electrostatic doping by applying a gate voltage. As a first step we have been able to fabricate phase-pure BBO on Nb-doped $SrTiO_3$ (STO) by pulsed laser deposition. High energy electron diffraction (RHEED) shows an island-like growth mode after formation of a wetting layer on the STO substrate, which may be due to the large lattice misfit of BBO and STO. A sharp low energy electron diffraction (LEED) pattern and X-ray diffraction evidence the epitaxial growth of crystalline BBO. In angle integrated photoemission experiments the samples reveal the valence band structure of cleaved undoped BBO single crystals. To our knowledge it is the first time that this could be shown on BBO thin films. Further experiments will elucidate the feasibility of doping electrons into these samples.

TT 103.40 Thu 15:00 Poster B

THz magneto-optics and FIR spectroscopy on topological insulators — •Nick Borgwardt[1], Gregor Mussler[2], Malte Langenbach[1], Joachim Hemberger[1], and Markus Grüninger[1] — [1]1 II. Physikalisches Institut, Universität zu Köln, Cologne, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany

Topological insulators are one of the most discussed areas of current research in condensed matter physics. Topological insulators show outstanding electromagnetic properties. One example is the Faraday rotation angle, which in the quantum Hall state is expected to be given by the fine structure constant. We report on optical data in the THz and FIR range measured on thin films of (Bi,Sb)2Te3 grown on high-resistive Si (111) wafers by MBE. For magneto-optical measurements in the THz range, we employ two photomixers placed inside a magneto-cryostat with magnetic fields B of up to 8T. Phase-sensitive detection of circularly polarized light allows for a direct determination of the Faraday rotation angle without any mechanically moving components in the THz path. We studied the transmittance and phase change as a function of temperature and magnetic field for thin films of various thicknesses.

TT 103.41 Thu 15:00 Poster B

XMCD of 3*d* adatoms on Bi_2Te_3 and Bi_2Te_2Se: experiment and *ab-initio* theory — Martin Vondráček[1], Malte Schüler[5], Markus Dunst[7], Cinthia Piamonteze[2], Jonas Warmuth[4], Matteo Michiardi[3], Lucas Barreto[3], Alexander Ako Khajetoorians[4,6], Jian-Li Mi[3], Bo B. Iversen[3], Philip Hofmann[3], Jens Wiebe[4], Tim Wehling[5], Jan Minár[7,8], Hubert Ebert[7], Roland Wiesendanger[4], and •Jan Honolka[1] — [1]Inst. of Physics ASCR, Prague, CZ — [2]PSI, CH — [3]iNano, Aarhus Univ., DK — [4]INF, Univ. of Hamburg, DE — [5]Inst. of Theo. Physics, Univ. of Bremen, DE — [6]Radboud Univ. Nijmegen, Inst. for Molec. and Mat., NL — [7]LMU München, DE — [8]Univ. of West Bohemia, CZ

The chalcogenide 3D topological insulator Bi_2Te_3 obeys time-reversal symmetry and hosts a linear dispersive, topological surface state around the Gamma point. It is predicted that magnetic adatoms can break time-reversal symmetry, thereby generating an energy gap at the Dirac point of the otherwise topologically protected surface states [1].

Here we summarize experimental XAS and XMCD results of single 3*d* adatoms Ni, Fe, and Cu on Bi_2Te_3 and Bi_2Te_2Se surfaces. While Cu shows a d^{10} electronic configuration, we find a significant resonant Ni $L_{2,3}$ intensity in XAS, however no magnetic dichroism within the detection limit. The results are compared to *ab-initio* theory. Calculated equilibrium positions of adatoms and their host structure show strong relaxation effects. *d*-shell occupancies and magnetic properties are extracted. Moreover, we present simulated resonant spectral shapes.

[1] Y. L. Chen et al., Science 329, 659 (2010).

TT 103.42 Thu 15:00 Poster B

Transport measurements on selective area grown Te-based topological insulator thin films — •Christian Weyrich[1,2], Melissa Schall[1,2], Jörn Kampmeier[1,2], Martin Lanius[1,2], Gregor Mussler[1,2], Thomas Schäpers[1,2], and Detlev Grützmacher[1,2] — [1]Peter Grünberg Institute (PGI- 9) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Virtual Institute for Topological Insulators (VITI), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

We present magnetotransport measurements on Bi_2Te_3 and Sb_2Te_3 thin films, grown on prepatterned structures atop silicon-on-insulator substrates by molecular beam epitaxy. The substrates contain Si mesa fabricated from the 70nm thick Si(111) top layer on a 300nm thick SiO_2 buried oxide layer. Therefore, we were able to utilize the difference in surface configuration between the Si(111) and the amorphous SiO_2, since only the hexagonal silicon surface supports growth of the tellurides. Using transport we show that films of comparable or even higher quality can be achieved using this method which furthermore evades the need of any additionally ex-situ patterning of the layers. With this, we pave the road to a simple fabrication method for nanometer sized structures that circumvents common problems of conventional methods like ion etching including hardened remains of photo resist and the like.

TT 103.43 Thu 15:00 Poster B

Individual tuning of the top and bottom surface states on a three dimensional topological insulator — •David Mahler, Jonas Wiedenmann, Cornelius Thienel, Kalle Bendias, Christopher Ames, Christoph Brüne, Hartmut Buhmann, and Laurens W. Mohlenkamp — Experimentelle Physik 3, Institut für Physik und Astronomie, Universität Würzburg

It has been shown, that the semimetal HgTe grown on a CdTe substrate becomes a three dimensional topological insulator due to its inverted band structure and the strain induced band gap of approximately 20 meV [1]. By using a top gate the dominance of the surface states in magneto transport data over a wide density range was observed and has been explained by the Dirac-screening of the surface states [2].

We demonstrate that the introduction of a back gate created by epitaxial growth on an n-doped gallium arsenide substrate allows us to

independently change the occupation of the upper and lower surface state. This can be shown by transport measurements at low temperatures and high magnetic fields. Therefore the occupation of the upper and lower surface state can be varied by the applied top and back gate voltages leading to different quantum hall sequences.

[1] C. Brüne et al., Phys. Rev. Lett. 106, 126803 (2011).
[2] C. Brüne et al., PRX to be published.

TT 103.44 Thu 15:00 Poster B

Quantum Anomalous Hall Effect in the presence of Rashba spin-orbit interaction — •Christoph Kleiner, Jan Boettcher, and Ewelina M. Hankiewicz — Universität Würzburg, Faculty for Physics and Astronomy

We study the quantum anomalous Hall (QAH) effect in $Hg_{1-y}Mn_yTe$ quantum wells. Here, the QAH effect occurs due to spin splitting in the presence of an intrinsic magnetisation which originates from the manganese atoms [1]. We use an effective four-band model (BHZ) in the tight-binding approximation to study the development of the spin splitting for the edge states and the bulk states. Increasing linearly the energy gap caused by the spin splitting leads to a non-linear behaviour for the bulk bands of one spin direction. Additionally, we observe, that the remaining edge state is shifted into the bulk bands of the opposite spin direction. Since there is no coupling between these two spin blocks in the BHZ model, there are crossings between these bulk bands and the edge states. Furthermore, we study the behaviour of the remaining edge state in the presence of Rashba spin-orbit interaction originating from an inversion breaking potential in the out of plane direction[2] which couples both spin blocks.

[1] Liu et al. PRL 101, 146802(2008).
[2] Rothe et al. New J. Phys. 12, 065012 (2010).

TT 103.45 Thu 15:00 Poster B

Transport at the edge of a 2D topological insulator — •Eslam Khalaf and Pavel Ostrovsky — Max Planck institute for solid state research, Stuttgart, Germany

We consider transport characteristics of the 2D topological insulator edge states in the presence of disorder. Two general setups are studied: a junction of the two quantum-Hall insulators and a relatively thick HgTe quantum well. In the first setup, an imbalance between the number of left- and right propagating modes (n_L and n_R) may occur at the interface if the filling factor is different on both sides of the junction. In this case, $|n_L - n_R|$ edge modes are topologically protected while all other states get eventually localized by disorder. If an edge of a thick HgTe quantum well carries an odd number of modes, one of them is also topologically protected from localization while others are localized at sufficiently long scales. For both systems, we compute the distribution of transmission probabilities and mesoscopic conductance fluctuations. Technically, this requires solving the one-dimensional non-linear sigma model with a topological term and source terms. The transfer-matrix formalism is employed which maps the problem to the problem of finding the eigenfunctions of Laplace operator on a symmetric superspace. For the quantum-Hall edge, the main effect of topology is the development of a gap in the transmission probability distribution around unit transmission for all length scales. In the case of HgTe quantum well, the probability distribution is also suppressed close to unit transmission but does not exhibit a hard gap.

TT 103.46 Thu 15:00 Poster B

Transport in topological insulator thin films: weak localization and universal conductance fluctuations — •Hristo Velkov[1,2], Georg Schwiete[1], and Tobias Micklitz[3] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz, 55128 Mainz, Germany — [2]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [3]Centro Brasileiro de Pesquisas Físicas, Rua Xavier Sigaud 150, 22290-180 Rio de Janeiro, Brazil

Motivated by the experimental difficulty to produce topological insulators with pure surface-state conduction, we study the effect that the bulk can have on the transport properties of the system. In particular, we focus on the weak localization (WL) and universal conductance fluctuations (UCF) physics in a topological insulator of the Bi_2Se_3 family, modelled by an effective low-energy Hamiltonian. Utilizing diagrammatic perturbation theory techniques we analyse the bulk and the surface separately and subsequently discuss WL and UCF when a tunneling-based coupling is introduced.

TT 103.47 Thu 15:00 Poster B

Microwave readout of Majorana qubits — •Christoph Ohm and Fabian Hassler — JARA Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

Majorana qubits offer a promising way to store and manipulate quantum information in a topologically protected way. Being immune to local noise the information is inherently hard to access rendering a measurement of the qubit state a challenging task. Here, we propose a readout scheme for Majorana qubits relying on the basic effect that voltage-biased Josephson junctions hosting Majorana fermions emit and absorb microwave photons at half of the Josephson frequency. Using standard tools from microwave engineering we show that in the dispersive regime our setup allows to perform a quantum non-demolition measurement and to reach the quantum limit. An appealing feature of our setup is that the interaction of the Majorana qubit with the measurement device can be turned on and off at will by changing the dc bias of the junction.

TT 103.48 Thu 15:00 Poster B

Magnetic order on a topological insulator surface with warping and proximity-induced superconductivity — •Daniel Mendler, Panagiotis Kotetes, and Gerd Schön — Institut für theoretische Festkörperphysik, Karlsruher Institut für Technologie

We determine the nature of the magnetic order on the surface of a topological insulator (TI) which develops due to hexagonal warping and the resulting Fermi surface (FS) nesting. By investigating the spin susceptibility and a microscopically-derived Landau theory, we explore the magnetic phases driven by a repulsive Hubbard interaction. We find that the magnetic ground state is formed by a superposition of three helical spin density waves which preserves C_3 symmetry. For a nearly hexagonal FS the magnetic ground state is topologically nontrivial with a non-zero skyrmionic charge. We show that the magnetic phase and the value of the skyrmionic charge can be controlled using magnetic fields and supercurrents. In addition, we explore the possibility of engineering a topological superconductor (TSC) when the TI is in proximity to a conventional SC and confirm the feasibility of an artificial C_3 symmetric TSC. We propose a technique to indirectly demonstrate the underlying skyrmion structure in the TSC, namely by measuring an induced multipolar distribution of supercurrents.

TT 103.49 Thu 15:00 Poster B

Majorana fermions from Shiba states in an antiferromagnetic chain on top of a superconductor — •Andreas Heimes, Panagiotis Kotetes, and Gerd Schön — Karlsruhe Institute of Technology

We propose a new mechanism for topological superconductivity based on an antiferromagnetically ordered chain of magnetic atoms on the surface of a conventional superconductor [1]. In a weak Zeeman field, a supercurrent in the substrate generates a staggered spin-current, which converts the preexisting topologically-unprotected Shiba states into Majorana fermions (MFs). The two experimental knobs can be finely tuned providing a platform with enhanced functionality for applications. Remarkably, the electronic spin-polarization of the arising edge MF wavefunctions depends solely on the parity of the number of magnetic moments, which can serve as a distinctive signature of the MFs. We introduce the basic concepts within a minimal model and make contact with experiments by a microscopic analysis based on the Shiba states.

[1] A. Heimes, P. Kotetes, and G. Schön,
Phys. Rev. B 90, 060507(R) (2014).

TT 103.50 Thu 15:00 Poster B

Majorana bound state coupled to helical edge states — •Daniel Frombach, Benedikt Probst, and Patrik Recher — Institut für Mathematische Physik, TU Braunschweig, 38106 Braunschweig, Germany

We investigate the coupling of a Majorana bound state (MBS) to helical edge states at the boundary of a two-dimensional topological insulator. We show that the transport properties of the helical edge states directly reflect the spin-direction of the MBS. We further investigate the reduced density matrix of a quantum bit built from four MBS coupled to helical edge states and discuss the influence of the different system parameters.

TT 103.51 Thu 15:00 Poster B

Optical detection of Majorana fermions via a quantum dot — •Luzie Weithofer, Anders Ström, and Patrik Recher — Insti-

tute of Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany

The search for Majorana bound states (MBS) in condensed matter systems is currently in the center of attention for theorists and experimentalists alike. Shortly after MBS have been predicted to emerge in "Majorana nanowires" [1,2], several experiments have indeed reported potential signatures of MBS. While these experiments concentrate on conductance measurements, here, we discuss the novel possibility of detecting MBS optically via their coupling to a quantum dot with a sufficiently strong dipole moment.

[1] Y. Oreg *et al.*, PRL **105**, 177002 (2010).
[2] J.D. Sau *et al.*, PRL **104**, 040502 (2010).

TT 103.52 Thu 15:00 Poster B

Correlations of weak measurements in a non-Markovian detection scheme — •Johannes Buelte[1], Adam Bednorz[2], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457, Germany — [2]Faculty of Physics, University of Warsaw, Hoza 69, PL-00681 Warsaw, Poland

Generalized quantum measurement schemes are described by positive operator-valued measures going beyond the projection postulate, which predicts the instantaneous collapse of the systems wave function. This allows to take the noninvasive limit and investigate the correlations of such weak measurements. We propose a scheme in which the detector is coupled to the measured system for a finite time, as it is the case in many real setups. This leads to non-Markovian effects, in accordance to the previous conjectures [1]. For the measured correlations this scheme predicts memory functions, which are related to symmetric and antisymmetric correlators of the detector variables. We investigate the memory functions under different general assumptions: (a) equilibrium detectors, (b) relation to the linear response Kubo formalism, (c) the role of non-equilibrium detectors and how they could realize the standard Markovian measurement. The latter scheme leads to the symmetrized operator order (aka Keldysh ordering), which is widely used in quantum measurement discussions.

[1] A. Bednorz , C. Bruder, B. Reulet, and W. Belzig,
Phys. Rev. Lett. 110, 250404 (2013)

TT 103.53 Thu 15:00 Poster B

Time-dependent factorial cumulants in quantum dots coupled to ferromagnetic leads — •Philipp Stegmann[1], Björn Sothmann[2], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [2]Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

Recently, theoretical studies have shown that factorial cumulants provide a useful tool to probe interaction in electronic transport through nanostructures [1, 2]. Sign changes of factorial cumulants as function of time indicate interaction, whereas in the absence of such sign changes the system can be described by an (effective) noninteracting Hamiltonian. We demonstrate this behavior for a quantum dot and for a mesoscopic Stoner particle [3] weakly tunnel coupled to two ferromagnetic leads.

[1] D. Kambly, C. Flindt, and M. Büttiker,
Phys. Rev. B **83**, 075432 (2011).
[2] D. Kambly and C. Flindt, J. Comput. Electron. 12, 331 (2013).
[3] B. Sothmann, J. König, and Y. Gefen,
Phys. Rev. Lett. **108**, 166603 (2012).

TT 103.54 Thu 15:00 Poster B

Highly resistive states in TiN wires induced by a high-impedance environment — •Ina Schneider[1], Tatyana Baturina[1,2], Klaus Kronfeldner[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]A.V. Rzhanov Institute of Semiconductor Physics SB RAS, Russia

We investigate different wires with similar aspect ratios, fabricated from a superconducting TiN thin film, at low temperatures and magnetic fields up to 15 T. The width of the wires varies between 20 nm and 1 μm. For the largest wires, we observe a typical superconducting behavior with a drop to zero resistance at sufficiently low temperatures and zero magnetic field. The medium sized wires show qualitatively similar $I(V)$- and $R(T)$-characteristics as the wide wires. However, their resistance does not drop to zero but saturates at finite values. For the smallest wire, the $R(T)$-characteristics reveal a slight increase of the resistance at zero field already.

By embedding the wires into a high impedance environment, we can induce a highly resistive state for the 80 nm wide wire, that manifests as a flat region in the $I(V)$-characteristics at very low bias voltages. This region starts to establish at magnetic fields where one could still observe a decrease of the resistance in the low-impedance environment measurements. At the peak of the magnetoresistance, this region corresponds to a resistance value which is by three orders of magnitude higher than that in the low-impedance environment.

TT 104: Topological Insulators II (jointly with MA, DS, HL, O)

Time: Thursday 15:00–17:45 Location: EB 202

TT 104.1 Thu 15:00 EB 202

Topological surface states of Heusler-type topological insulators — •Shu-Chun Wu[1], Binghai Yan[1,2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Max Planck Institute for Physics of the Complex Systems, Dresden, Germany

Some promising half-Heusler compounds, *R*PtBi (R = La, Lu, Y), are demonstrated experimentally to be superconductors and are predicted to be topological insulators. The topological feature of bulk is band inversion and the *s* orbital of Pt atom is the main clue. However, their topological surface states (TSSs) remain unclear. In this work, we use *ab initio* method to investigate the TSSs. In experiment, they are found at the Γ point inside the valence bands. Spin texture is also calculated to confirm the topologically nontrivial surface states. External strain can push the TSSs from the valence bands up into gap.

TT 104.2 Thu 15:15 EB 202

Topological surface states on NaBaBi with two opposite spin textures — •Yan Sun[1], Shu-Chun Wu[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany. — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany.

By breaking the inversion symmetry of the 3D Dirac metal Na_3Bi, we realize topological insulator (TI) phases in a known compound NaBaBi using $ab-initio$ calculations. Two distinct TI phases emerge: one phase is due to the band inversion between $Bi-p$ and $Na-s$ bands, and the other phase (under pressure) is induced by the inverted $Bi-p$ and $Ba-d$ bands. Both phases exhibit Dirac-cone-type surface states, but opposite spin textures. In the upper cone, a left-hand spin texture exists for the s-p inverted phase (similar to a common TI, e.g. Bi_2Se_3) while a right-hand spin texture appears for the $p-d$ inverted phase. NaBaBi presents a prototype model for TIs that exhibit different spin textures in the same material.

TT 104.3 Thu 15:30 EB 202

Indirect exchange interaction through topological surface states in crystalline topological insulators of a SnTe class — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

As predicted theoretically [1,2] and confirmed experimentally [2,3] the interface of SnTe and vacuum (i.e. the material's surface) hosts topologically stable Dirac states. We investigate the properties of this state within a **k.p** model that includes a full account of the bulk band structure [4]. An essential advantage of an analytical band model [4] is that it allows to unequivocally trace the two key degrees of freedom that this system possesses: spin and pseudospin. The indirect exchange interaction between magnetic impurities is a perfect probe for the surface Dirac states, especially for their spin structure. We revealed explicitly the dependence of this interaction on the properties of the bulk band states, in particular on the spin orbit coupling strength and on the crystal field splitting parameters. Depending on these parameters, the interaction may be either of Ising type or of a novel anisotropic XY type with the spin direction aligned with the connection vector

between the two impurities.
[1] B.A. Volkov, and O.A. Pankratov, *JETP Lett.* **42**, 178, 1985.
[2] T.H. Hsieh *et al.*, *N*ature Comm. **3**, 982, 2012.
[3] Y. Tanaka *et al.*, *N*ature Phys. **8**, 800, 2012.
[4] B.A. Volkov, and O.A. Pankratov, *Z*h.Eksp. Theor. Fiz. **75**, 1362, 1978.

TT 104.4 Thu 15:45 EB 202

Edge states in topological magnon insulators — Alexander Mook[1], •Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle (Saale), Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

For magnons, the Dzyaloshinskii-Moriya interaction accounts for spin-orbit interaction and causes a nontrivial topology that allows for topological magnon insulators. In this theoretical investigation [1] we present the bulk-boundary correspondence for magnonic kagome lattices by studying the edge magnons calculated by a Green function renormalization technique. Our analysis explains the sign of the transverse thermal conductivity of the magnon Hall effect in terms of topological edge modes and their propagation direction. The hybridization of topologically trivial with nontrivial edge modes enlarges the period in reciprocal space of the latter, which is explained by the topology of the involved modes.

[1] Phys. Rev. B **90** (2014) 024412.

TT 104.5 Thu 16:00 EB 202

Magnon waveguides from topological magnon insulators — •Alexander Mook[1], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle

Topological magnon insulators exhibit a nontrivial topology due to the Dzyaloshinskii-Moriya interaction. They host topologically nontrivial edge magnons and, consequently, energy as well as spin currents along their edges [1,2].

Bringing two topological magnon insulators into contact results in topologically protected unidirectional interface magnons. As these interface modes decay toward both bulk regions, their currents are confined to a few nanometer wide strip around the interface. Owing to the topological nature of the edge states, the edge currents follow any geometry.

We address theoretically the formation of interface edge magnons and their currents. On top of this, we propose recipes to compose magnon waveguides with nano-scale confinement.

[1] L. Zhang et al., PRB **87**, 144101 (2013).
[2] A. Mook et al., PRB **90**, 024412 (2014).

TT 104.6 Thu 16:15 EB 202

Probing the Electronic Properties of Individual MnPc Molecules Coupled to Topological States — •Thomas Bathon[1], Paolo Sessi[1], Konstantin Kokh[2], Oleg Tereshchenko[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik 2, Universitaet Wuerzburg, Am Hubland, 97074 Wuerzburg, Germany — [2]Novosibirsk State University, 630090 Novosibirsk, Russia

Hybrid organic-inorganic interfaces have been widely reported to host emergent properties that go beyond those of their single constituents. Coupling molecules to the recently discovered topological insulators, which possess linearly dispersing and spin-momentum-locked Dirac fermions, may offer a promising platform towards new functionalities.

Here, we report a scanning tunneling microscopy and spectroscopy study of the prototypical interface between MnPc molecules and a Bi_2Te_3 surface. MnPc is found to bind stably to the substrate through its central Mn atom. The adsorption process is only accompanied by a minor charge transfer across the interface, resulting in a moderately n-doped Bi_2Te_3 surface. More remarkably, topological states remain completely unaffected by the presence of the molecules, as evidenced by the absence of scattering patterns around adsorption sites. Interestingly, we show that, while the HOMO and LUMO orbitals closely resemble those of MnPc in the gas phase, a new hybrid state emerges through interaction with the substrate.

TT 104.7 Thu 16:30 EB 202

first principle study of structural, electronic and magnetic properties of graphene nanoribbons deposited on the topological insulator Sb2Te3 — wei zhang[1,2], •farideh hajiheidari[1], yan li[1,3], manuel j. schmidt[1], and riccardo mazzarello[1,4] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52074 Aachen, Germany — [2]Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [3]IEK-6, Forschungszentrum Jülich, D-52425 Jülich, Germany — [4]JARA-FIT and JARA-HPC, RWTH Aachen University, D-52074 Aachen, Germany

Magnetic perturbations are known to affect the surface properties of a topological insulator (TI) dramatically. According to mean-field calculations, zigzag graphene nanoribbons (zGNRs) possess spin-polarized edge states. Hence, zGNRs deposited on a TI could be a promising candidate for an experimental investigation of proximity effects between a magnetic system and a TI. In this work, we carry out a first-principles investigation based on density functional theory of zGNRs on the Sb2Te3 (001) surface. We use gradient-corrected density functionals in combination with semi-empirical van der Waals corrections. Both H-free and H-terminated zGNRs are considered. In the case of H-free zGNRs, the strong interaction between the edge atoms and the TI surface is shown to lead to the bending of the zGNRs , however, the edge magnetism is preserved. Moreover, the magnetic anisotropy axis is perpendicular to the surface of the substrate. In the H-terminated case, on the other hand, the interaction is less significant and edge magnetism is fully preserved.

TT 104.8 Thu 16:45 EB 202

WSe_2 Synthesis, Characterization and Properties — •Catherine R Rajamathi, Binghai Yan, Marcus Schmidt, Kumari Gaurav Rana, Chandra Shekhar, Siham Ouardi, Guido Kreiner, and Claudia Felser — Max-Planck Institute for Chemical Physics of Solids, Dresden

Layered transition metal dichalcogenides (TMDs) are widely studied systems as they are chemically versatile and technologically enthralling. The facile tunability of their electronic structure by varying certain parameters - carrier type (n- or p-type), composition, structure or sample size expand their applications from catalysis to topological insulators. Single crystals were synthesized from its polycrystalline components using $SeCl_4$ as the transport agent. Mono- or few-layered tungsten selenide obtained by the scotch-tape technique discussed in this talk are direct-gap semiconductors. FET devices fabricated from a few-layered sample of WSe_2 show ambipolar transistor behavior. In addition, hybrid materials such as $WSe_{2-x}Te_x$ may be promising due to high magnetoresistance and surface states on WTe_2 single crystals.

TT 104.9 Thu 17:00 EB 202

Classification of spin liquids on the square lattice with strong spin-orbit coupling — •Johannes Reuther[1,2], Shu-Ping Lee[3], and Jason Alicea[3] — [1]Freie Universität Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie — [3]California Institute of Technology

The investigation of spin liquids is a fascinating field in condensed matter physics that is increasingly motivated by experiments. Exhaustive classifications of spin liquids have been carried out in several systems, particularly when full SU(2) spin-rotation symmetry is present. Systematic studies that explore strongly spin-orbit-coupled magnetic compounds (for which there are many experimental examples) are, however, relatively scarce. We report on a classification of Z_2 spin liquids on the square lattice when SU(2) spin symmetry is maximally lifted. Using projective symmetry group methods, we find that, surprisingly, the lifting of spin symmetry yields vastly more spin liquid states compared to SU(2)-invariant systems. A generic feature of the SU(2)-broken case is that the spinons naturally undergo $p + ip$ pairing; consequently, many of these Z_2 spin liquids feature a topologically nontrivial spinon band structure supporting gapless Majorana edge states. These boundary modes are often protected by a combination of time reversal and lattice symmetries and hence resemble recently proposed topological crystalline superconductors.

TT 104.10 Thu 17:15 EB 202

Fate of the 1/3 magnetization plateau in quantum triangular antiferromagnets with various anisotropies — •Fedor Simkovic[1], Natasha Perkins[2], and Andrey Chubukov[2] — [1]King's College, London, England — [2]University of Minnesota, Minneapolis, United States

The triangular Heisenberg lattice is investigated by means of semi-classical 1/S expansion. Although classically the up-up-down phase with 1/3 magnetisation exists only at one magnitude of the field, it is

stabilised by quantum fluctuations and forms a magnetisation plateau around this point. We investigate into three types of anisotropies for the triangular lattice, and access the stability of the aforementioned phase towards the limits of decoupled chains, the square, honeycomb, Kagome, rhombille and scaled triangular lattices.

TT 104.11 Thu 17:30 EB 202

Matrix product operators: Local equivalences and topological order in 2D — •Oliver Buerschaper — Freie Universität Berlin

Projected entangled pair states (PEPS), which naturally generalize matrix product states (MPS) to higher dimensions, describe the low energy properties of local quantum Hamiltonians with an energy gap very well. For this reason they are increasingly used as a valuable tool in both analytical and numerical studies of strongly correlated 2D quantum systems. Some of the most interesting such systems exhibit topological order, i.e. patterns of long-range entanglement which cannot be detected by any local order parameter. At the same time, excitations in these systems typically exhibit fractional statistics and may be used, for instance, as a resource for topological quantum computation.

For both fundamental and practical reasons, it is thus of the utmost importance to understand and classify PEPS in 2D, especially those with topological order. Recently it was found that symmetries defined in terms of certain matrix product operators (MPO) provide a mechanism for the emergence of topological order in PEPS. Furthermore, the kind of topological order was seen to depend on the algebraic properties of the given MPO symmetry. Here we show that many, seemingly distinct MPO symmetries are, in fact, locally equivalent and characterize PEPS with the *same* kind of topological order. We discuss interesting ramifications for the classification of 2D quantum systems.

TT 105: Quantum Information Systems: Si Vacancies and NV Centers (jointly with HL)

Time: Thursday 15:00–17:00 Location: ER 164

TT 105.1 Thu 15:00 ER 164

Spin Physics of vacancy-related defects in silicon carbide — •Michel Bockstedte[1,2] and Felix Schütz[1] — [1]Lst. Theor. Festkörperphysik, Friedrich-Alexander Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]FB Materialwissenschaften & Physik, Universität Salzburg, 5020 Salzburg, Austria

SiC as a semi conductor fullfills all necessary requirements[1] for implenting qubits via defect electron spins, such as the silicon vacancy, the di-vacancy or a complex of a silicon vacancy and a nitrogen impurity. The spin-selective fluorescence in contrast to the prototypical NV-center in diamond operates in the spectral range favorable for telecom applications. Spin-manipulation of the intrinsic centers was demonstrated even at room temperature.[2,3] For the silicon vacany in SiC inter system crossings (ISCs) from high to yet unknown low spin states govern the spin-relaxation. By DFT and a DFT-based CI-hamiltonian we analyze the spin physics of the defect in 4H-SiC. Experimentally observed luminescence lines can be assigned to the inequivalent defect sites corobarating the experimental findings. Owing to the spin (S=3/2) and a stronger electron-phonon coupling in the excited state, ISCs destinct from the NV-center are predicted.

[1] J. R. Weber *et al.*, PNAS **107**, 8513 (2010).
[2] F. Koehl *et al.*, Nature**479**, 84 (2011).
[3] V. A. Soltamov *et al.*, Phys. Rev. Lett. **108** 226402 (2012)

TT 105.2 Thu 15:15 ER 164

SiC nano-crystalline NIR emitters based on optically excited and spin polarized defects — •F. Fuchs[1], A. Muzha[2], N. Tarakina[3,4], D. Simin[1], M. Trupke[5], P. Baranov[6], V. Dyakonov[1,3,7], A. Krueger[2,3], and G. Astakhov[1] — [1]Exp. Physics VI, University of Würzburg — [2]Institute of Organic Chemistry, University of Würzburg — [3]Wilhelm Conrad Röntgen RCCM, University of Würzburg — [4]Exp. Physics III, University of Würzburg — [5]Vienna Center for Quantum Science and Technology, TU Wien — [6]Ioffe Institute, St. Petersburg — [7]ZAE Bayern, Würzburg

The unification of luminescent markers for bioimaging and spin centers for quantum sensing [1] is challenging; especially when aiming for the ideal NIR window, stability and non-toxicity. Bulk silicon carbide (SiC) is a favored candidate despite its large band gap, which we could mitigate by the introduction of silicon vacancy defects—exhibiting NIR emission—via neutron irradiation. With a milling procedure, we fabricated SiC nano crystals ranging from 600nm down to 60nm in size, with a further fragmentation of the latter into clusters of high crystalline quality (size ca. 10 nm) separated by amorphous material. The luminescence of the vacancies persists in all size fractions, moreover, we detected room-temperature spin resonance [2]. This leads to new perspectives: defects in nano crystalline SiC as in-vivo luminescent markers and simultaneously as magnetic field or temperature sensors [3].

[1] Riedel et al.: Phys. Rev. Lett. 109, 22 (2012)
[2] Fuchs et al. arXiv: 1409.0756v1
[3] Kraus et al.: Sci. Rep. 4, 5303 (2014)

TT 105.3 Thu 15:30 ER 164

Coherent Spin Manipulation of Si-Vacancies in Silicon Carbide at Ambient Conditions — •Dmitrij Simin[1], Andreas Sperlich[1], Victor Soltamov[2], Pavel Baranov[2], Georgy Astakhov[1], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Wuerzburg, 97074 Wuerzburg — [2]Ioffe Physical-Technical Institute, 194021 St. Petersburg, Russia — [3]ZAE Bayern, 97074 Wuerzburg

For already over two decades, quantum information processing has been the hot topic in the field of information theory. To recognize and to employ the most suitable material and information carrier from the vast amount of possibilities is the declared goal of ongoing research activities all over the world. Among others, a promising candidate are Si-vacancies in Silicon Carbide [1], where spin control has been successfully conducted at ambient conditions [2, 3]. In our recent work we go one step further and present the successful time-resolved manipulation of the spin of the Si-Vacancies at ambient conditions using the pulsed-ODMR technique. We observed Rabi-oscillations in an ensemble of defects and determined spin-relaxation properties, demonstrating high potential of SiC for various quantum applications.

[1] D. Riedel et al., Phys. Rev. Lett. 109, 226402 (2012)
[2] H. Kraus et al., Nat. Phys. 10, 157-162 (2014)
[3] H. Kraus et al., Sci. Rep. 4, 5303 (2014)

TT 105.4 Thu 15:45 ER 164

Charge state control of nitrogen-vacancy centers in diamond — •Patrick Simon[1], Moritz V. Hauf[1], Ankit Rathi[1], Philipp Neumann[2], Helmut Fedder[2], Jörg Wrachtrup[2], Friedemann Reinhard[1,2], and Jose A. Garrido[1] — [1]Walter Schottky Institut, Physik-Department,Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [2]3. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

The nitrogen-vacancy (NV) defect in diamond is a promising candidate for quantum information processing or sensing purposes. In most applications reliable control of the charge state of the NV is of utmost importance.

In this work we demonstrate that the charge state of NV centers can be controlled using an in-plane gated diamond nanostructure based on selective surface termination. Applying a gate voltage changes the band bending at the hydrogen terminated diamond surface such that reversible charge state switching is enabled. We observed full control of NVs from a non-fluorescent state, potentially NV^+, across NV^0 to NV^-

TT 105.5 Thu 16:00 ER 164

Investigating the positively charged nitrogen-vacancy center in diamond as a long lived quantum memory — •Matthias Pfender[1], Nabeel Aslam[1], Christian Burk[1], Denis Antonov[1], Sebastian Zaiser[1], Helmut Fedder[1], Philipp Neumann[1], Patrick Simon[2], José A. Garrido[2], Martin Stutzmann[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart — [2]Walter Schottky Institut, Technische Universität München

The nitrogen-vacancy defect in diamond is one of the major candidates for a solid-state quantum processor. Its electron spin can be readout and initialized optically. Adjacent nuclear spins (e.g. ^{14}N,

^{15}N, ^{13}C) can be employed as inherently robust qubits [1], readout is facilitated via the electron spin in a QND measurement with T_1 lifetimes of several minutes. However, for strongly coupled nuclear spins, the coherence time is limited by the T_1 lifetime of the electron spin ($\approx$ 5ms). In Si:P, this obstacle could be overcome by ionizing the P donor to a spinless charge-state [2]. In this work, we employ in-plane gate structures to deterministically switch the charge state of near-surface NVs from NV^- over NV^0 to NV^+ [3], while investigating the electron spin properties using the nitrogen nuclear spin as a probe. Since the positive charge state has no unpaired electrons, the nuclear spin coherence time is prolonged beyond the 5ms imposed by the NV^- electron spin.

[1] Waldherr, G. et al., Nature 506, 204 (2014).
[2] Saeedi, K. et al., Science 342, 830 (2013).
[3] Hauf, M. V. et al., Nano Lett. 14, 2359 (2014).

TT 105.6 Thu 16:15 ER 164

A cavity-mediated quantum CPHASE gate between nitrogen-vacancy electronic spin qubits in diamond — •Guido Burkard[1] and David Awschalom[2] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637, USA

While long spin coherence times and efficient single-qubit quantum control have been implemented successfully in nitrogen-vacancy (NV) centers in diamond, the controlled coupling of remote NV spin qubits remains challenging. Here, we propose and analyze a controlled-phase (CPHASE) gate for the spins of two NV centers embedded in a common optical cavity and driven by two off-resonant lasers. In combination with previously demonstrated single-qubit gates, CPHASE allows for arbitrary quantum computations. The coupling of the NV spin to the cavity mode is based upon Raman transitions via the NV excited states and can be controlled with the laser intensities and relative phase. We find characteristic laser frequencies at which a laser photon is only scattered into the cavity mode if the NV center spin is $|m_s = 0\rangle$, and not in the case $|m_s = -1\rangle$, or vice versa. The scattered photon can be reabsorbed by another selectively driven NV center and generate a conditional phase (CPHASE) gate. Gate times below 20 ns are within reach, several orders of magnitude shorter than typical NV spin coherence times. The separation between the two NV centers is only limited by the extension of the cavity.

[1] G. Burkard, D. D. Awschalom, arXiv: 1402.6351 (2014).

TT 105.7 Thu 16:30 ER 164

Long-range two-qubit gate between nuclear spins in diamond mediated via an optical cavity — •Adrian Auer and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

Nitrogen-vacancy (NV) centers in diamond represent a promising possibility for a solid-state based realization of a qubit due to their excellent electron- and nuclear-spin coherence properties. Single-qubit gates for the nitrogen nuclear spin have been implemented [1]. Here, we extend an earlier proposal [2] for cavity-mediated coupling between NV electron spins and develop a scheme to implement a universal two-qubit gate between ^{14}N or ^{15}N nuclear spins. By virtually exciting a single NV center with an external laser field, a photon can be scattered into a surrounding cavity; we show that this process depends on the spin state of the nitrogen nucleus. For the two-qubit gate, we consider two NV centers coupled to a common cavity mode and each being excited individually. Virtual cavity excitation can then mediate an effective interaction between the NV nuclear spin qubits, generating a controlled-Z gate. Operation times for the gate implementation are found to be below 100 nanoseconds, which is orders of magnitude faster than the decoherence time of nuclear spin qubits in diamond.

[1] S. Sangtawesin *et al.*, Phys. Rev. Lett. **113**, 020506 (2014).
[2] G. Burkard and D. D. Awschalom, arXiv:1402.6351.

TT 105.8 Thu 16:45 ER 164

Linear polarization properties of the NV^- center photoluminescence in diamond — •Dion Braukmann[1], Jörg Debus[1], Vladimir L. Korenev[2], Vitalii Yu. Ivanov[3], Dmitri R. Yakovlev[1], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Science, 194021 St. Petersburg, Russia — [3]Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland

The negatively charged nitrogen-vacancy (NV^-) center in diamond has been studied in recent years on account of possible applications in quantum information processing, spin-electronics and, e.g., biophotonics. Particular focus has been drawn onto its optical properties. We report on polarization-dependent optical studies of NV^- centers in diamond subjected to high magnetic fields of up to 10 T. We observe asymmetric Zeeman splitting of the zero-phonon line photoluminescence, a strong optical alignment as well as Faraday rotation at room temperature. The linear polarization properties of the NV^- photoluminescence are studied as function of the diamond crystal orientation in the stationary and time-resolved regimes.

TT 106: Frontiers of Electronic Structure Theory: Many-Body Effects, Methods (organized by O)

Time: Thursday 15:00–18:30 Location: MA 004

Invited Talk TT 106.1 Thu 15:00 MA 004

Natural orbital functional theory with higher-order occupation probabilities — •Ralph Gebauer[1], Roberto Car[2], and Morrel Cohen[2,3] — [1]International Centre for Theoretical Physics (ICTP), Trieste, Italy — [2]Department of Chemistry, Princeton University, Princeton, USA — [3]Department of Physics and Astronomy, Rutgers University, USA

We introduce a novel energy functional for ground-state electronic-structure calculations. Its fundamental variables are the natural spin-orbitals of the implied singlet many-body wave function and their joint occupation probabilities. The functional derives from a sequence of controlled approximations to the two-particle density matrix. Algebraic scaling of computational cost with electron number is obtainable in general, and Hartree-Fock scaling in the seniority-zero version of the theory. Results obtained with the latter version for saturated small molecular systems are compared with those of highly-accurate quantum-chemical computations. The numerical results are variational, capturing most of the correlation energy from equilibrium to dissociation. Their accuracy is considerably greater than that obtainable with current density-functional theory approximations and with current functionals of the one-particle density matrix only.

TT 106.2 Thu 15:30 MA 004

Electronic Properties of Surfaces and Interfaces with Self-Consistent Interatomic van der Waals Density Functional — •Nicola Ferri[1], Robert A. Distasio Jr.[2], Alberto Ambrosetti[1], Roberto Car[2], Matthias Scheffler[1], and Alexandre Tkatchenko[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Princeton University, USA

Ubiquitous long-range van der Waals (vdW) interactions play a fundamental role in the structure and stability of a wide range of systems. Within the DFT framework, the vdW energy represents a crucial, but tiny part (0.001%) of the total energy, hence its influence on the electronic density, $n(\mathbf{r})$, and derived electronic properties is typically assumed to be rather small. Here, we address this question via a fully self-consistent (SC) implementation of the interatomic Tkatchenko-Scheffler vdW functional [1] and its extension to surfaces [2]. For several transition metal surfaces, self-consistency increases their dipole moments and induces non-trivial electron density rearrangements. As a consequence, we observed changes of up to 0.3 eV in the surface work-functions, with vdW self-consistency improving the agreement with experiments. Similar behavior is observed for molecules adsorbed on metals, where vdW contributions influence both Pauli push-back and charge transfer, the two phenomena that determine interface work-functions. [1] A. Tkatchenko and M. Scheffler, PRL (2009). [2] V. G. Ruiz, W. Liu, E. Zojer, M. Scheffler, and A. Tkatchenko, PRL (2012).

TT 106.3 Thu 15:45 MA 004

Exact functionals for a lattice model — •Tanja Dimitrov[1], Heiko Appel[1,3], and Angel Rubio[1,2,3] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Nano-bio Spectroscopy Group/ETSF Scientific Development Centre, Universidad del Pais Vasco UPV/EHU, San Sebastian — [3]MPI for the Structure and Dynamics of Matter, Hamburg

Standard local exchange-correlation and semi-local functionals in ground-state density functional theory are known for their shortcomings in describing correct charge transfer, dissociation energies of molecular ions, and barriers of chemical reactions [1,2]. To understand the failures of approximate functionals, to gain insight into the behavior of the exact functional, and to devise new approximations, we investigate the exact solution of the many-body Schrödinger equation in Fock space for a lattice model with a softened Coulomb interaction term. Using quadratic optimization with quadratic constraints, or alternatively exact diagonalization, we explicitely construct the *exact* density-to-potential and density-to-wave-function map. We discuss the behavior of functionals in the low-density limit.

[1] A. J. Cohen et al. Science **321**, 792 (2008).
[2] P. Mori-Sanchez et al., Phys. Rev. Lett. **100**, 146401 (2008).

TT 106.4 Thu 16:00 MA 004

Many-body dispersion meets non-local density functionals: A unified approach for van der Waals correlations — •Jan Hermann, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

It is an ongoing challenge to develop an efficient method for van der Waals (vdW) non-local correlation within DFT which would be both accurate and broadly applicable. Current approaches can be loosely divided into the fragment-based ones, two-point density functionals and methods based on the density-density response function. The fragment-based models utilize parameters not derivable from the electron density. Two-point approaches are explicit density functionals, but difficult to generalize to include many-body correlations.

Here, we show that these seemingly contrasting approaches can be unified within a single framework based on the adiabatic-connection formalism in the random-phase approximation. We use a local response-function model from the VV09 functional [1] together with the many-body dispersion approach to create an atom-based model with no external parameters. We introduce a consistent correlation-functional-based coupling of the short- and long-range correlation energy. We show that this unification provides new insights into the different approaches, naturally deals with the partitioning of ionic and delocalized states and paves path towards self-consistent description of many-body vdW correlations.

[1] O. A. Vydrov, T. Van Voorhis, Phys. Rev. Lett. 103, 063004

TT 106.5 Thu 16:15 MA 004

Reduced Density-Matrix Functional Theory: correlation and spectroscopy — Stefano Di Sabatino[1], Jan A. Berger[2], Lucia Reining[3], and •Pina Romaniello[1] — [1]Laboratoire de Physique Théorique, CNRS, IRSAMC, Université Toulouse III - Paul Sabatier, Toulouse, France and ETSF — [2]Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université Toulouse III - Paul Sabatier, CNRS, Toulouse, France and ETSF — [3]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, Palaiseau, France and ETSF

We study the performance of approximations to electron correlation in reduced density-matrix functional theory (RDMFT) and of approximations to the observables calculated within this theory [1]. We use the exactly solvable Hubbard molecule as test case. In particular we focus on the atomic limit and we explore how degeneracies and spin-symmetry breaking are treated in RDMFT. We find that, within the used approximations, RDMFT is not able to describe the signature of strong correlation in the spin-singlet ground state, whereas it give the exact result for the spin-symmetry broken case. [1] S. Di Sabatino, J.A. Berger, L. Reining, and P. Romaniello, submitted

TT 106.6 Thu 16:30 MA 004

Does *GW* obey the straight-line condition? — Matthias Dauth[1,3], Fabio Caruso[2], Stephan Kuemmel[1], and •Patrick Rinke[3] — [1]University of Bayreuth, Germany — [2]University of Oxford, England — [3]Aalto University, Helsinki, Finland

Many-body theory in the *GW* approach has become the method of choice for calculating charged excitations in solids. Recently, it is also increasingly being applied to molecules, but fundamental questions regarding its accuracy remain. One such fundamental theorem requires that the total energy changes linearly with gradual (i.e. fractional) ionisation of the molecule. In this work we investigate, if *GW* is piecewise linear or if it exhibits a derivation of the straight line error (DSLE). Since the derivative of the total energy with respect to the electron number gives the ionisation energy, we quantify the DSLE by taking the difference between the energy of the highest occupied state of the neutral and the lowest unoccupied state of the singly ionised molecule (which would be equal in the DSLE-free case). We find for a subset of molecules from the quantum chemical G2 benchmark set, that the DSLE in self-consistent *GW* amounts to 1.1 eV on average. This DSLE can be mitigated in perturbative G_0W_0 by varying the starting point. We use density-functional theory as starting point and vary the amount of exact exchange α in the Perdew-Burke-Ernzerhof hybrid functional (PBEh). G_0W_0 becomes DSLE-free for $\alpha \approx 0.4$. The average deviation from the experimental IPs is then very close to that of self-consistent *GW* and amounts to ∼0.25 eV.

TT 106.7 Thu 16:45 MA 004

Green's Function embedding for Advanced Electronic Structure Methods based on Dynamical Mean-Field Theory — •Wael Chibani[1], Xinguo Ren[2], Matthias Scheffler[1], and Patrick Rinke[3] — [1]*Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany* — [2]*Key Laboratory of Quantum Information, USTC, Hefei, China* — [3]*Aalto University, Helsinki, Finland*

We introduce an embedding scheme for periodic systems that facilitates a self-consistent treatment of the physically important part of a system with electronic structure methods, that are computationally too expensive for periodic systems. We use dynamical mean-field theory [1] (DMFT) to couple to the rest of the system, which is treated with less demanding approaches such as Kohn-Sham density functional theory. In contrast to the original DMFT formulation for correlated model Hamiltonians, we consider here the unit cell as local embedded cluster in an *ab initio* way, that includes all electronic degrees of freedom. The performance of our scheme is demonstrated by treating the embedded region with hybrid and *GW* self-energies (sc*GW*) for simple bulk systems. The total energy and the density of states converge rapidly with respect to the computational parameters and approach their bulk limit with increasing cluster size. For non self-consistent *GW* calculations we observe Plasmon satellites for Si – in good agreement with periodic G_0W_0 calculations [2] – that vanish at self-consistency. Our sc*GW* gap of ∼ 0.9 eV for a two atom unit cell agrees well with previous G_0W_0 calculations and experiment. [1] A.Georges *et al.*, Rev.Mod.Phys.(2006), [2] M.Guzzo *et al.*, PRL(2011)

TT 106.8 Thu 17:00 MA 004

Improved Ground State Electronic Structure and Optical Dielectric Constants With a Semi-Local Exchange Functional — •Vojtěch Vlček[1], Gerd Steinle-Neumann[1], Linn Leppert[1], Rickard Armiento[2], and Stephan Kümmel[1] — [1]University of Bayreuth, Germany — [2]Linköping University, Sweden

For a set of solids, we explore a recently developed generalized gradient exchange functional (AK13) that has two characteristic features: its enhancement factor diverges for large reduced density gradients s as $s \ln(s)$ and its potential changes discontinuously at integer electron numbers. We apply the functional to semiconductors, Mott insulators, and ionic crystals and compare results for band structure and dielectric constants with a standard GGA. The AK13 functional provides a better description of the KS orbitals and we observe a qualitative improvement both in the bandgaps and in the optical dielectric constants, especially for the small gap semiconductors we explore (Ge, α-Sn, and CdO)

TT 106.9 Thu 17:15 MA 004

Accurate, efficient localized resolution of identity of the Coulomb operator across the periodic table — •Arvid Ihrig[1], Jürgen Wieferink[1], Igor Ying Zhang[1], Patrick Rinke[1,2], Volker Blum[1,3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Aalto University, Helsinki, Finland — [3]Duke University, Durham, USA

A key component of advanced electronic structure methods is the explicit evaluation of the Coulomb operator. The corresponding four-center integrals can be solved with a "resolution of identity" (RI) approach for numeric atom-centered orbitals, as they are used in, e.g., FHI-aims [1]. In RI, basis function products are expanded in an auxiliary basis. The complete auxiliary basis is used for "RI-V", the most accurate and most commonly used RI. We developed a localized RI ("RI-LVL"), which expands the products only in the subset of those auxiliary functions centered on the same atoms as the basis functions.

This approach yields a superior scaling with system size, both in terms of computational time and memory requirements. At the same time it also retains the accuracy of the RI-V, as we have shown for HF, MP2, PBE0 and RPA calculations. The systems we investigated include weakly interacting molecular dimers (S22 test set) as well as TiO_2, Cu, and Au clusters. In all test cases we found that RI-LVL reproduces RI-V very accurately. Even for RPA-calculations of gold with very large basis sets the deviation to RI-V is only ∼1.5 meV per atom. [1] V. Blum *et al.*, Comput. Phys. Commun. **180**, 2175 (2009).

TT 106.10 Thu 17:30 MA 004

Explicitly correlated self consistent field theory — •Christian Lasar and Thorsten Klüner — Carl von Ossitzky Universität, Oldenburg, Germany

There is a variety of methods available which aim to describe molecules and molecular reactions with chemical accuracy. The two main classes of these methods are density functional theory (DFT) and electron correlation approaches. DFT achieves great accuracy for many molecules and is applicable to quite large molecules. Unfortunately, DFT is not systematically improvable since the exact form of the exchange correlation functional remains unknown. Correlation methods do not suffer from this lack of systematic improvement. Unfortunately, they often require too much computational resources for large molecules. Additionally, they show a very slow convergence with the size of the basis set. Explicitly correlated methods are known to be able to solve this convergence problem. In these methods, the wavefunction is augmented with a function f_{ij} which explicitly depends on two electronic coordinates. Combining the advantages of low computational resources and the ability for systematic improvement, one ends up in the following ansatz for the wavefunction $\Psi = (1 + \sum_{ij} f_{ij})\Phi$, where Φ is one slater determinant. With this ansatz the long determinant expansion is avoided. Additionally, there will be a fast convergence with the basis set size. We currently investigate the derivation of the working equations and their implementation for different functions f_{ij}. Some results for small molecules have already been obtained and will be presented in this contribution.

TT 106.11 Thu 17:45 MA 004

Comparison of two self-consistent *GW* schemes — •Peter Koval[1], Dietrich Foerster[2], and Daniel Sanchez-Portal[1,3] — [1]Donostia International Physics Center, San Sebastián, Spain — [2]Laboratoire Ondes et Matiére d'Aquitaine, Bordeaux, France — [3]Material Physics Center, San Sebastián, Spain

GW approximation (*GW*A) as a competitor of DFT provides a better description of electronic structure in several respects. However, a *GW* calculation is more expensive than similar DFT calculation. This fact contributed to a wide usage of simpler calculations based on *GW*A (SEX, COSEX, plasmon-pole approximations etc.) This manyfold of approximations hampers a non-biased evaluation of merits of *GW*A to describe the electronic correlations. We produced a rigorous *GW* implementation where the only approximation is the use of localized orbitals [1]. The usage of spectral functions allowed us to realize two self-consistent *GW* schemes: sc*GW* [2] and qs*GW* [3] in one code [4]. Furthermore, we used all-electron Gaussian basis sets that allows for a coherent comparison with quantum chemistry methods. We use coupled-cluster methods CCSD and CCSD(T) as reference and compare ionization potentials of 15 molecules. The calculations show trends in sc*GW* and qs*GW* and give hints on possible sources of discrepancies/directions towards improving *GW*A. [1] D. Foerster, P. Koval, D. Sánchez-Portal, *J. Chem. Phys.* **135**, 074105 (2011); [2] L. Hedin, *J. Phys. Cond. Mat.* **11**, R489 (1999); [3] S. V. Faleev, M. van Schilfgaarde, T. Kotani, *Phys. Rev. Lett.* **93**, 126406 (2004); [2] P. Koval, D. Foerster, D. Sánchez-Portal, *Phys. Rev.* B **89**, 155417 (2014).

TT 106.12 Thu 18:00 MA 004

Quasiparticle Self-Consistent *GW* for Molecules — •Ferdnand Kaplan[1,2,3], Michiel van Setten[1,2,5], Florian Weigend[1,3], and Ferdinand Evers[1,2,3,4] — [1]Institute of Nanotechnology (INT) — [2]Institute for Theoretical Condensed Matter Physics (TKM) — [3]Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [4]Universität Regensburg, D-93040 Regensburg, Germany — [5]Université catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium

One of the most used approaches for the computational study of nanoscale systems and molecules is the density functional theory (DFT). However, DFT calculations of single particle excitation spectra, e.g. ionization potentials, often suffer from method-inherent difficulties. To systematically improve the estimation of quasi-particle energies for molecular system, we have implemented the *GW* method. The approach represents a perturbative expansion of the many-body Green's function with respect to the screened Coulomb interaction, W.

On G_0W_0 level the *GW*-self energy is calculated with the Kohn-Sham Green's function of the underlying DFT. Hence, one finds a strong dependence of the excitation energies on the reference system, i.e. DFT functionals. To overcome this problem, we implemented a self-consistent cycle which takes into account the deviations of the quasiparicle(qp)-wavefunctions from their Kohn-Sham parents.

We find that this procedure converges to a fixed point solution which is independent of the reference system. For the testset of molecules anlyzed by us so far, the results for ionization-energy and electron-affinity improve upon G_0W_0, when comparing to experimental data.

TT 106.13 Thu 18:15 MA 004

Pure state N-representability conditions: Should they be taken into account in Reduced density matrix functional theory? — •Iris Theophilou[1], Nektarios Lathiotakis[2,3], and Nicole Helbig[1] — [1]Peter Grünberg Institut (PGI-1), Forschungszentrum Jülich, Jülich, Gernany — [2]Theoretical and Physical Chemistry Institute (TPCI), National Hellenic Research Foundation , Athens, Greece — [3]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

In Reduced Density Matrix Functional Theory (RDMFT) the natural occupation numbers are minimized under the ensemble N-representability conditions, i.e they are restricted to be between zero and one and sum to the number of electrons. Recently, the pure state N-representability problem for the one-body reduced density matrix has been solved [M. Altunbulak and A. Klyachko, Commun. Math. Phys. 282, 287 (2008)]. In this talk we discuss to which extend these pure state conditions are satisfied without being enforced in 3 electron systems using some standard RDMFT functionals. Our aim is to impose those pure state conditions that are not automatically satisfied and check whether this improves RDMFT results.

TT 107: Graphene: Electronic Structure (jointly with O, HL)

Time: Thursday 15:00–18:15 Location: MA 041

TT 107.1 Thu 15:00 MA 041

Tuning the electronic structure of artificial graphene with potential modulation — •Pilkwang Kim and Cheol-Hwan Park — Department of Physics, Seoul National University, Seoul 151-747, Korea

Among the many different directions of research for tuning the electronic properties of massless Dirac fermions residing in materials like graphene, one of the promising candidates is the artificial graphene system where a conventional two-dimensional electron gas is modulated by external periodic potential, as first predicted theoretically [1,2]. Recently, experimentalists have confirmed the existence of massless Dirac fermions originating from metallic surface states [3,4]. In this presentation, we discuss our theoretical study on the possibility of tuning the electronic properties of massless Dirac fermions residing in 2DEG by exploiting the external potential degree of freedom. This work was supported by Korean NRF funded by MSIP (Grant No. NRF-2013R1A1A1076141).

[1] C.-H. Park and S. G. Louie, Nano Lett. 9, 1793 (2009).

[2] M. Gibertini, A. Singha, V. Pellegrini, M. Polini, G. Vignale, A. Pinczuk, L. Pfeiffer, and K. West, Phys. Rev. B 79, 241406 (2009).

[3] K. K. Gomes, W. Mar, W. Ko, F. Guinea, and H. C. Manoharan, Nature 483, 306 (2013).

[4] S. Wang, L. Z. Tan, W. Wang, S. G. Louie, and N. Lin, Phys. Rev. Lett. 113, 196803 (2014).

TT 107.2 Thu 15:15 MA 041

Using collective electrostatic effects to tune the electronic

structure of graphene — •Gernot J. Kraberger[1], David A. Egger[1,2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel

Graphene has unique structural and electronic properties, which have attracted huge research interest since its isolation. As a prerequisite of using this material in devices, it is necessary to modify its properties in a controlled way that it fits the needs of the application. This work uses density functional theory calculations to investigate a new approach to change the electronic structure of graphene: using the collective field of a highly ordered arrangement of dipoles to shift the potential in specific regions of graphene (i.e., exploiting so-called collective electrostatic effects). First we discuss a "proof-of-concept" model system: Along a line in graphene, pairs of neighboring carbon atoms are replaced by a boron and a nitrogen atom. Each of the resulting BN-pairs exhibits a dipole moment, which means that a one-dimensional chain of dipoles is formed. This chain impacts the electrostatic potential in its surroundings such that the electronic states in graphene are locally shifted relative to the Fermi level. With two oppositely oriented lines of dipoles it is then even possible to localize states in well-defined stripes. Finally, we explore to what extent similar effects can be generated by assembling rows of quadrupolar molecules on top of the graphene sheet instead of modifying the graphene layer itself.

TT 107.3 Thu 15:30 MA 041

Graphene on weakly interacting metals: Dirac states vs. surface states — •Wouter Jolie, Fabian Craes, and Carsten Busse — II. Physikalisches Institut, Universität zu Köln, Germany

The epitaxial growth of graphene and other two-dimensional materials on metal surfaces has become a well-established procedure and is extensively used for studies of the electronic properties of two-dimensional materials using surface science methods. However, the substrate itself can have a significant contribution to these properties. We demonstrate this on three different systems: graphene on a thick silver film on Ir(111), graphene on one monolayer of silver on Ir(111), and graphene on Ir(111). We explore the interplay between the states of the substrate (in form of nearly free surface states) and the states of the two-dimensional material on top (in form of graphenes' Dirac fermions) with scanning tunneling spectroscopy, a technique sensitive to the local density of states of the surface. We show that, when present, the surface state represents the dominant contribution in form of Friedel oscillations and confined states on graphene quantum dots. We compare these findings with a system with suppressed surface states where a clear feature of graphene is found in the density of states.

TT 107.4 Thu 15:45 MA 041

Size quantization effects in quasiparticle interference on epitaxial graphene nanoflakes — •Julia Tesch[1], Philipp Leicht[1], Felix Blumenschein[1], Anders Bergvall[2], Tomas Löfwander[2], Luca Gragnaniello[1], and Mikhail Fonin[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Chalmers University of Technology, Göteborg, Sweden

Graphene nanostructures represent an exciting topic for research, as a strong spatial confinement together with the edge structure impose new electronic properties, making them promising candidates for future nanoscale electronic units. Here, we investigate by means of low-temperature scanning tunnelling microscopy and spectroscopy oblong quasi-freestanding epitaxial graphene nanoflakes prepared on Ag(111) and Au(111) by intercalation with virtually no edge bonding [1]. We implement quasiparticle interference (QPI) mapping to analyze standing wave patterns arising from elastic scattering processes within a single nanoflake. The Fourier analysis of the obtained QPI maps shows that in addition to ringlike structures due to the *intervalley* and *intravalley* scattering observed for large graphene sheets, additional scattering features are visible, which can be related to the transverse modes in a nanoflake [2]. Our experimental results are supported by tight-binding calculations of realistic flakes, which very well reproduce the experimentally observed fingerprints of confinement in the Fourier transform of the standing wave patterns.

[1] P. Leicht *et al.*, ACS Nano **8**, 3735 (2014); [2] A. Bergvall *et al.*, Phys. Rev. B **87**, 205431 (2013).

TT 107.5 Thu 16:00 MA 041

Graphene-supported metal clusters: A two photon photoemission study — Kira Jochmann and •Thorsten Bernhardt — Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm

During the last decade considerable attention was drawn to the growth of graphene on metal single crystal surfaces, where it provides an ideal template for the ordered growth of regular metal cluster arrays. Building on various investigations about the detailed growth of these cluster super-lattices, we make use of the possibility to easily grow nanostructures with equally spaced and mono-disperse clusters for fundamental research in laser selective photochemistry. Our new experimental setup enables time-resolved measurements due to a femtosecond laser system on the one hand and surface analysis via scanning tunnelling microscopy on the other hand. In first light interaction measurements time-resolved two-photon photoemission spectroscopy (2PPES) was applied to gain an insight into the unoccupied electronic structure of the Ir(111)/graphene/Ir cluster system at different graphene and cluster coverages. In subsequent experiments the combination of femtosecond laser pump-probe mass spectrometry with resonance enhanced multi-photon ionization and STM will be employed to reveal photo-dissociation dynamics of different adsorbate molecules with spatio-temporal resolution.

TT 107.6 Thu 16:15 MA 041

From ribbons to constrictions: STM lithography on ballistic sidewall graphene nanoribbons — •Jens Baringhaus[1], Mikkel Settnes[2], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Technical University of Denmark, DTU Nanotech, Center for Nanostructured Graphene (CNG), 2800 Kgs. Lyngby, Denmark

The selective graphene growth on the sidewalls of SiC mesa structures produces well-ordered graphene nanoribbons (GNR) with exceptional transport properties. Using a 4-tip STM, a probe spacing and temperature independent conductance of e^2/h is found, indicating single channel ballistic transport even at room temperature [1]. The robustness of the ballistic channel makes these GNR ideal templates for morphological alterations. For this purpose, one of the STM tips is used for local lithography. Careful control over the feedback parameters and the bias voltage allows to either fully cut the ribbon or to create narrow, a few nm wide constrictions. Every STM lithography step is monitored directly by local transport. After a full cut, the transport characteristics of the sidewall GNR are completely destroyed. In contrast, in narrow constrictions the ballistic channel is preserved, but only present at bias voltages exceeding 10 mV. Additionally, localized currents manifest as resonances in the IV curves at bias voltages of about 8 mV. Using a standard tight binding and recursive Green's function approach, the resonances are found to be robust against temperature as well as different types of disorder, e.g. Anderson or edge disorder.

[1] Baringhaus et al., Nature **506**, 349 (2014)

TT 107.7 Thu 16:30 MA 041

Chiral Enhanced Phonon Spectroscopy of Graphene — •Fabian D. Natterer[1], Yue Zhao[1,2], Jonathan Wyrick[1], Wen-Ying Ruan[3], Yang-Hao Chan[4], Mei-Yin Chou[3,4], Nikolai B. Zhitenev[1], and Joseph A. Stroscio[1] — [1]Center for Nanoscale Science and Technology, NIST, Gaithersburg, USA — [2]University of Maryland, College Park, USA — [3]Georgia Institute of Technology, Atlanta, USA — [4]Academia Sinica, Taipei, Taiwan

In graphene, many phenomena are driven by the interaction with phonons, such as the relaxation of hot carriers or the mediation of many-body interactions. The proper characterization of phonons can therefore shed important insights into graphene based devices. Such devices were characterized by inelastic electron tunneling spectroscopy (IETS) but weak signals and other spectral features obscured a clear distinction between phonons and miscellaneous excitations. In this talk, I show that we are able to map large parts of the graphene phonon density of states by using a back gated graphene device, where the charge carrier density can be varied in magnitude and sign. Our averaging technique combines individual IETS data, obtained over the entire charge carrier range, with the benefit of improving the signal for inelastic excitations. Surprisingly, we observe that the graphene phonon intensity is enhanced when the charge carrier type is switched, indicating that this amplification occurs whenever the inelastic transition allows a change in the graphene chirality. The chiral enhancement follows a linear trend with energy and reaches almost an order of magnitude for the highest mode.

TT 107.8 Thu 16:45 MA 041

Luminescence of Graphene in the Visible Spectral Range af-

ter Short-Pulse Excitation in the Near Infrared — •Martin Rothe, Günter Kewes, Nikolai Severin, Jürgen P. Rabe, and Oliver Benson — Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, D-12489 Berlin, Germany

Graphene is well known for its unique electronic and optical properties. The study and manipulation of its nonlinear optical response at energies in the range of visible light is of interest for the understanding of its charge carrier dynamics in this energy regime [1]. We find a broad luminescence of graphene and graphene multilayers in the entire visible spectral range after excitation with fs laser pulses in the near infrared. The spectrum that starts even above twice the excitation energy indicates multi-photon absorption or efficient electron scattering processes. This method of luminescence excitation is not only well suited for imaging with high contrast but can also gain insight into fundamental electron relaxation and collective excitation processes [2].

[1] Liu, et al., Phys Rev B: 82, 081408 (2010)
[2] Lange, et al., arXiv:1404.6518 (2014)

TT 107.9 Thu 17:00 MA 041

Electroluminescence from carbon-based nanostructures — •Ji Hoon Ryoo and Cheol-Hwan Park — Department of Physics, Seoul National University, Seoul 151-747, Korea

Light emission from carbon nanostructures upon current flowing reflects their novel electronic structures and is important for applications purposes. Peculiar emission versus photon energy profiles in the electroluminescence from carbon nanostructures have been attributed to inter-band electronic transitions [1], electron-phonon interactions [2] and interference effects [3]. In this presentation, we discuss the origin of multi-peak intensity versus energy feature in the electroluminescence from graphene based on recent experimental results, and look into how the electronic structure of graphene affects its electroluminescence. This work was supported by Korean NRF funded by MSIP (Grant No. NRF-2013R1A1A1076141). Computational resources have been provided by Aspiring Researcher Program through Seoul National University (SNU) in 2014.

[1] D. Mann, Y. K. Kato, A. Kinkhabwala, E. Pop, J. Cao, X. Wang, L. Zhang, Q. Wang, J. Guo, H. Dai, Nature Nanotech. 2, 33-38 (2007).
[2] S. Essig, C. W. Marquardt, A. Vijayaraghavan, M. Ganzhorn, S. Dehm, . Henrich, F. Ou, A. A. Green, C. Sciascia, F. Bonaccorso, K.-P. Bohnen, H. v. Löhneysen, M. M. Kappes, P. M. Ajayan, M. C. Hersam, A. C. Ferrari, R. Krupke, Nano Lett. 10, 1589-1594 (2010).
[3] M. Engel, M. Steiner, A. Lombardo, A. C. Ferrari, H. v. Löhneysen, P. Avouris, R. Krupke, Nature Comm. 3, 906 (2012).

TT 107.10 Thu 17:15 MA 041

Structure and electronic states of the zig-zag graphene/h-BN interface — •Robert Drost[1], Andreas Uppstu[2], Kezilebieke Shawulienu[1], Fabian Schulz[1], Sampsa K. Hämäläinen[1], Mikko Ervasti[2], Ari Harju[2], and Peter Liljeroth[1] — [1]Department of Applied Physics, Aalto University School of Science, Finland — [2]COMP Centre of Excellence and Helsinki Institute of Physics, Department of Applied Physics, Aalto University School of Science, Finland

Some of the most exciting properties of graphene (G) are only realised in atomically precise nanostructures. The zig-zag (ZZ) edges of this two-dimensional crystal host localised states that have been proposed to be used in spin- and valleytronic applications: Using the spin degree of freedom of the electron or the valley degree of freedom of the honeycomb crystal structure to transmit and process information. While well studied theoretically, experimental realisations remain challenging. We passivate the ZZ edge of epitaxial G with hexagonal boron-nitride (BN), a 2D insulator isostructural to G, to preserve the edge state in the band gap of the insulator. We investigate the growth of atomically perfect G/BN heterostructures on Ir(111) and Ni(111) substrates and discuss the effect of varying substrate interaction. The intrinsic properties of the G/BN interface may be revealed by intercalation with gold. Using low-temperature STM, we demonstrate the existence of a localised electronic state on the ZZ oriented G/BN interfaces. Tight binding and DFT calculations show that the interface retains many important properties of the graphene edge state.

TT 107.11 Thu 17:30 MA 041

Embedding graphene quantum dots into hexagonal boron nitride — Ferdinand Farwick zum Hagen[1], Caio Silva[1], Christoph Schlueter[2], Nicolae Atodiresei[3], Wouter Jolie[1], Daniela Dombrowski[1], Antonio J. Martinez-Galera[1], Domenik Zimmermann[1], Ulrike Schröder[1], Vasile Caciuc[3], Thomas Michely[1], Stefan Blügel[3], Tien-Lin Lee[2], and •Carsten Busse[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Diamond Light Source, Didcot, UK — [3]Peter Grünberg Institute, Forschungszentrum Jülich, Germany

Graphene (gr) nanostructures can be stabilized by embedding them into an insulating matrix. Hexagonal boron nitride (hBN) is especially suited as it is isostructural to graphene, and dangling C bonds can be satisfied by B and N. In this study, we used sequential epitaxial growth of gr and hBN on Ir(111) to embed graphene quantum dots (GQDs).
First, we investigate pristine hBN/Ir(111) with special attention to the hBN-substrate interaction which is characterized by the local varying layer height as determined with x-ray standing waves (XSW), complemented by density functional theory (DFT) calculations. Distinct differences with respect to gr/Ir(111) are found: A stronger corrugation within the moiré and an enhanced chemical interaction in the strongly bound parts of the supercell. Second, the edge atoms of GQDs on Ir(111) are investigated and an enhanced C-substrate interaction is found. Third, the chemical and structural changes at these edges upon embedding in hBN are probed. The in-plane structure is analyzed using scanning tunneling microscopy (STM).

TT 107.12 Thu 17:45 MA 041

Single 3*d* transition metal atoms on multi-layer graphene systems: electronic configurations, bonding mechanism and role of the substrate — Violetta Sessi[6], Sebastian Stepanow[1,2], Alexander N. Rudenko[3], Sören Krotzky[1], Klaus Kern[1], Fanny Hiebel[4], Pierre Mallet[4], Jean-Yves Veuillen[4], Ondřej Šipr[5], •Jan Honolka[1,5], and Nick B. Brookes[6] — [1]Max-Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]Department of Materials, ETH Zürich, Switzerland — [3]Radboud University Nijmegen, Inst. for Molecules and Materials, Netherlands — [4]Institut Néel, CNRS-UJF, Grenoble, France — [5]Inst. of Physics, ASCR, Prague, Czech Republic — [6]ESRF, Grenoble, France

We present our recent study on electronic configurations of Fe, Co, Ni and Cu adatoms on graphene and graphite by x-ray magnetic circular dichroism and charge transfer multiplet theory [1]. A delicate interplay between long-range interactions and local chemical bonding is found to influence the adatom equilibrium distance and magnetic moment. The results for Fe and Co are consistent with purely physisorbed species having, however, different 3*d*-shell occupations on graphene and graphite (d^{n+1} and d^n, respectively). On the other hand, for the late 3*d* metals Ni and Cu a trend towards chemisorption is found, which strongly quenches the magnetic moment on both substrates.

[1] V. Sessi et al., New J. of Physics 16, 062001 (2014) [Fast Track Communication]

TT 107.13 Thu 18:00 MA 041

Ab initio **calculation of XNLD in reflection of graphene** — •Dominik Legut[1], Peter M. Oppeneer[2], Christine Jansing[3], Marc F. Tesch[3,4], Markus Gilbert[3], Andreas Gaupp[3], Hans-Christoph Mertins[3], Andrey Sokolov[4], Suk-Ho Choi[5], Hud Wahab[6], Heiko Timmers[6], and R.G. Elliman[7] — [1]IT4Innovations Centre, VSB-TU Ostrava, Ostrava, Czech Republic — [2]Department of Physics and Astronomy, Uppsala, Sweden — [3]FH Münster, Steinfurt, Germany — [4]HZB, Berlin, Germany — [5]Department of Applied Physics, Kyung Hee University, Korea — [6]University of New South Wales Canberra, Canberra BC, Australia — [7]Department of Elect. Mat. Eng., Australian National University, Canberra, Australia

The reflection spectroscopy and in particular angular dependence of the x-ray natural linear dichroism (XNLD) were calculated on free standing monolayered graphene. The anisotropic XNLD was computed in the single electron picture within the framework of the DFT. The excitations stemming from carbon K-edge are considered. The spectral shape of the XNLD is compared with recorded data. The dependence of the reflection spectroscopy, here XNLD, based on the change of the electronic structure of bi-layer and tri-layered graphene is predicted.

TT 108: Spin-Dependent Transport Phenomena II (organized by MA)

Time: Thursday 15:00–18:00 Location: H 0112

TT 108.1 Thu 15:00 H 0112

D'yakonov-Perel' spin dephasing in metallic films — •N. H. Long, P. Mavropoulos, D. S. G. Bauer, B. Zimmermann, Y. Mokrousov, and S. Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The D'yakonov-Perel' mechanism for spin dephasing of conduction electrons is prominent in systems with broken space-inversion symmetry, where spin-orbit coupling induces a **k**-dependent Zeeman-type field, the *spin-orbit field* $\mathbf{\Omega_k}$. The electron spin precesses around $\mathbf{\Omega_k}$, while momentum scattering into a different state $\mathbf{k'}$ results in a new precession axis $\mathbf{\Omega_{k'}}$, eventually leading to spin dephasing. The mechanism is well-studied in semiconductors but not in metals that usually have inversion symmetry, which is, however, lifted in metallic films deposited on a substrate.

In this work we employ density-functional theory and a linear response approach for the calculation of the spin-orbit fields in supported metallic films typically used in spintronics, such as Au(111) or Pt(111). A kinetic equation is applied to derive the dephasing time that is found to be smaller than the Elliott-Yafet spin-relaxation time, e.g., 100 ns in 24-layer Au(111) films with self-adatom impurities. We discuss the importance of the mechanism in systems of varying film thickness and impurity concentration.

We acknowledge funding from the DFG SPP-1538 SpinCaT and HGF-YIG Programme VH-NG-513.

TT 108.2 Thu 15:15 H 0112

Description of magneto-optics of disordered alloys from first principles — •Kristina Chadova[1], Rudolf Sykora[2], Dominik Legut[2], Diemo Ködderitzsch[1], Hubert Ebert[1], and Jan Minár[1,3] — [1]Department of Chemistry, Physical Chemistry, Ludwig-Maximilians University Munich, Germany — [2]Nanotechnology Centre VSB - Technical University of Ostrava, 17. Listopadu 15/2172, 708 33 Ostrava-Poruba, Czech Republic — [3]NewTechnologies-Research Center, University of West Bohemia, Pilsen, Czech Republic

The optical properties of pure - as well as disordered - alloys have received a lot of interest as they play an important role, for example in storage applications. We present a first-principle approach to calculate magneto-optical properties based on the Kubo formula implemented within the fully relativistic KKR (Korringa-Kohn-Rostoker) formalism in combination with coherent potential approximation accounting for chemical disorder in substitutional random alloys. The implemented formalism allows to calculate the full frequency dependent conductivity tensor and to discuss on this basis the magneto-optical effects. The first results will be presented for ferromagnetic transition metal alloys.

TT 108.3 Thu 15:30 H 0112

Compton profiles of random $Fe_{0.5}Ni_{0.5}$ alloy, evidence for the interplay of disorder and correlation in momentum space — •Liviu Chioncel[1,2], Diana Benea[3,4], Hubert Ebert[4], and Jan Minar[4,5] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D - 86135 Augsburg, Germany — [2]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [3]Faculty of Physics, Babes-Bolyai University, Kogalniceanustr 1, Ro-400084 Cluj-Napoca, Romania — [4]Chemistry Department, University Munich, Butenandstr. 5-13, D-81377 München, Germany — [5]New Technologies - Research Center, University of West Bohemia, Univerzitni 8, 306 14 Pilsen, Czech Republic

We study the magnetic Compton profile of the disordered $Fe_{50}Ni_{50}$ alloy and discuss the interplay between structural disorder and electronic correlations. The disorder distribution is described within the Coherent Potential Approximation while local electronic correlations are captured with the Dynamical Mean Field Theory. The disorder induced changes in the experimental magnetic Compton profiles are well described by the theoretical calculations only when both components Fe and Ni are subject to considerable electronic correlations.

TT 108.4 Thu 15:45 H 0112

Current Induced Domain Wall Depinning in Non-Local Spin Valve Half Ring Structures — •Alexander Pfeiffer[1], William Savero Torres[2], Nils Richter[1], Laurent Vila[2], Jean Philippe Attané[2], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]Institut Nanosciences et Cryogénie, Université Grenoble Alpes & CEA, France

We demonstrate current induced domain wall depinning and phase transitions in non-local spin valve Permalloy/Aluminium half ring structures. With our optimized geometry by patterning a notch acting as a pinning center in one half ring, we are to able study the influence of Oersted fields, Joule heating and the spin transfer torque. We find a complete depinning event at zero applied external field for a charge current density of 600 GA/m^2, showing that our geometry can be used for low power domain wall manipulation.

TT 108.5 Thu 16:00 H 0112

Electronic transport from ab-inito linear response – a generalized Kubo-Bastin approach — •Diemo Ködderitzsch, Kristina Chadova, and Hubert Ebert — Department Chemie, Ludwig-Maximilians-Universität, 81377 München, Germany

Starting from a Kubo-Bastin like linear response expression we present a general approach to describe various linear response phenomena from ab-inito. Within a fully relativistic KKR framework in a spin-density functional formulation we treat among other things the full (spin-) conductivity tensor including its antisymmetric components and thereby spin-orbit induced transverse transport phenomena like the spin- and anomalous Hall effects. Both Fermi-sea and Fermi-surface terms are described on the same footing. Employing the coherent potential approximation allows to treat, besides pure systems, disordered alloys through the whole concentration range. Within this approach intrinsic as well as extrinsic contributions are fully accounted for without any model assumptions. In this context the role of vertex corrections and their importance will be discussed. Applications to transition-metals and their alloys will be presented.

15 min. break

TT 108.6 Thu 16:30 H 0112

Transverse transport and magneto-optical properties of non-collinear antiferromagnets — •Sebastian Wimmer, Ján Minár, Sergiy Mankovsky, Diemo Ködderitzsch, and Hubert Ebert — Ludwig-Maximilians-Universität München, München, Deutschland

Recently, a number of investigations on the anomalous Hall effect (AHE) in materials having nontrivial spin structures, such as non-collinear antiferromagnets, have been performed [1-4]. One especially striking result is the prediction of the AHE for a system with zero net magnetization [3]. We revisit and extend these studies employing a combined group theoretical and first principles approach.

Based exclusively on symmetry considerations the occurence of transverse transport and related optical effects for a given magnetic order of a solid can be predicted. Numerical studies using a first principles electronic structure method in the framework of Korringa-Kohn-Rostoker (KKR) multiple scattering theory and subsequent calculation of response quantities using a Kubo-type linear response formalism are performed to independently cross-check the group theoretical predictions. Our results in part confirm previous findings and furthermore give first numerical estimates of the magnitude of magneto-optical properties experimentally not observed so far.

[1] S. Yoshii, S. Iikubo, T. Kageyama, K. Oda, Y. Kondo, K. Murata, and M. Sato, JPSJ **69**, 3777 (2000). [2] T. Tomizawa and H. Kontani, PRB **82**, 104412 (2010). [3] H. Chen, Q. Niu, and A. H. MacDonald, PRL **112**, 017205 (2014). [4] J. Kübler and C. Felser, arXiv:1410.5985 [cond-mat.mtrl-sci] (2014).

TT 108.7 Thu 16:45 H 0112

Sign change in tunnel magnetoresistance of Fe_3O_4/MgO/CoFeB magnetic tunnel junctions depending on annealing temperature and interface treatment — Luca Marnitz[1], Karsten Rott[1], Stefan Niehörster[1], Christoph Klewe[1], Daniel Meier[1], Savio Fabretti[1], Matthäus Witziok[2], Andreas Krampf[2], Olga Schuckmann[2], Tobias Schemme[2], Karsten Kuepper[2], Joachim Wollschläger[2], Andy Thomas[1], Günter Reiss[1], and •Timo Kuschel[1] — [1]CSMD, Physics Department, Bielefeld University, Germany — [2]Physics Department, Osnabrück University, Germany

Magnetite (Fe_3O_4) is a promising candidate for magnetic tunnel junc-

tions (MTJs) since it shows a high spin polarization at the Fermi level as well as a high Curie temperature of 585°C. However, MTJs with magnetite electrodes have not shown a large tunnel magnetoresistance (TMR) so far. It is reported in literature for magnetite on MgO that Mg^{2+} ions diffuses into the magnetite at growth temperatures above 250°C, replacing parts of the Fe^{2+} ions. In typical magnetite MTJs MgO is used both as substrate as well as barrier material.
In this study, a sign change in the TMR of Fe_3O_4/MgO/CoFeB MTJs is observed after annealing at temperatures between 200°C and 280°C which can be explained by Mg interdiffusion from the MgO barrier into the magnetite. Additionally, different treatments of the magnetite interface during the preparation of the MTJs have been studied regarding their effect on the performance of the MTJs. A maximum TMR of up to -12% was observed despite exposing the magnetite surface to atmospheric conditions prior to the deposition of the MgO barrier.

TT 108.8 Thu 17:00 H 0112

Tunneling Anisotropic Magnetoresistance in oxide heterostructures — •Nico Homonnay[1], Johannes Lotze[1], Robert Göckeritz[1], Alexander Müller[1], Tim Richter[1], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

We have investigated tunneling anisotropic magnetoresistance (TAMR) [1] in hybrid structures consisting of an epitaxial stack of a ferromagnetic oxide ($La_{0.7}Sr_{0.3}MnO_3$, LSMO) and an oxide tunnel barrier ($SrTiO_3$, STO) fitted with a non-magnetic metal contact. The oxide stack was deposited by pulsed laser deposition and metallization was done without breaking UHV conditions using various metals for different samples. The layers were processed to vertical tunneling devices with lateral dimensions of approx. 10 μm and the devices were investigated at low temperature in a 4He bath cryostate equipped with a 3D vector magnet. In all devices we observe TAMR which strongly depends on temperature, bias voltage and thickness of the tunnel barrier. The TAMR signal can be larger than 50 % which is more than 10 times bigger than reported for inorganic systems [1]. The magnetoresistance is clearly identified as TAMR by in-plane magnetic field sweeps at different angles. The TAMR signal persists up to a bias voltage of approx. 1 V and up to a temperature of 240 K which is well below the Curie temperature of the LSMO. [1] Gould et al., Phys. Rev. Lett. 93, 117203 (2004)

TT 108.9 Thu 17:15 H 0112

Spin-dependent Fano effect and two-stage Kondo effect in T-shaped double quantum dots with ferromagnetic leads — •Krzysztof P. Wójcik and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland

We analyze the influence of ferromagnetism of the leads on the transport properties of T-shaped double quantum dots. The calculations are performed by using the numerical renormalization group method. We focus on two particularly interesting phenomena occurring in such systems: the Fano-like interference causing a strong antiresonance in the dependence of the linear conductance on the gate voltage, and the two-stage Kondo effect. The latter effect is related with a nonmonotonic dependence of the linear conductance on temperature T: with lowering T below the Kondo temperature the conductance is first enhanced, but then at the second stage it becomes suppressed due to the formation of spin singlet state between two singly occupied quantum dots. We find that spin-resolved tunneling can suppress the second stage of the Kondo effect for appropriately chosen dots' energy levels. Moreover, we show that the presence of ferromagnets results in spin-dependent conditions for the Fano destructive interference, which gives the possibility of tuning the spin polarization of the linear conductance in the range $[-1, +1]$.

TT 108.10 Thu 17:30 H 0112

The influence of Coulomb interactions on spin-dependent thermoelectric transport through double quantum dot system with Rashba spin-orbit coupling — •Łukasz Karwacki and Piotr Trocha — Faculty of Physics, Adam Mickiewicz University, Poznań, Poland

We investigate theoretically a double quantum dot system embedded into an Aharonov-Bohm ring and coupled to two electronic reservoirs. The magnetic potential present in the system due to the Aharonov-Bohm device leads to spin-independent phase factors in terms related to coupling between the dots and the electrodes. Furthermore, we assume additional spin-dependent phase factors arising from Rashba spin-orbit interaction. We show the influence of the aforementioned phases and that of the Coulomb blockade on the dots on such basic thermoelectric parameters as charge and spin conductances, electronic contribution to heat conductance, charge and spin thermopower and the resulting thermoelectric effectiveness factor.

In our approach we focus on the linear response regime, where the thermoelectric parameters are functions of transmission coefficient. To derive this coefficient we employ equation of motion for non-equilibrium Green's function method.

The results indicate a possibility for an efficient spin-dependent Seebeck generator. Tuning the Rashba spin-orbit interaction leads to pure spin current through the system. In both cases Coulomb blockade leads to enhancement of thermoelectric transport.

TT 108.11 Thu 17:45 H 0112

Tunable Thermoelectric Power Factors of Magnetoresistive Nanowires — •Anna Niemann[1], Tim Böhnert[1], Ann-Kathrin Michel[1], Svenja Bässler[1], Johannes Gooth[1], Bence G. Tóth[2], Katalin Neuróhr[2], László Péter[2], Imre Bakonyi[2], Victor Vega[3], Victor M. Prida[3], and Kornelius Nielsch[1] — [1]Universität Hamburg, Hamburg, Germany — [2]Hungarian Academy of Sciences, Budapest, Hungary — [3]Universidad de Oviedo, Oviedo, Spain

We present spin-caloric transport in single Co-Ni alloy and multilayered Co-Ni/Cu nanowires, including magnetoresistance (MR) and magneto-thermopower (MTP) measurements. Co-Ni alloy nanowires show anisotropic MR while multilayered nanowires show predominant giant MR. MTP and MR are studied in a temperature range between 50 K and 325 K leading to effect sizes up to 6 % for Co-Ni alloy samples and up to 15 % for multilayered samples at room temperature. While the thermopower describes a material's ability to convert temperature gradients into electrical voltage, thermoelectric power factors (PFs) give a measure of the electrical power generated from thermoelectric effects. The PFs of our nanowires can compete with common thermoelectric bulk materials like Bi_2Te_3. Additionally, a magnetic field-dependence of the nanowires' PFs can be observed. PFs of Co-Ni nanowires increase by 24 % in an external magnetic field, while PFs of multilayered nanowires can be increased by up to 40 %. This magnetic field dependence opens interesting opportunities to tune electrical power output according to applicational needs.

TT 109: Transport: Majorana Fermions (jointly with DS, HL, MA, O)

Time: Friday 9:30–12:15 Location: H 0104

TT 109.1 Fri 9:30 H 0104

Majorana bound states in a Corbino geometry topological insulator Josephson junction — •Sunghun Park and Patrik Recher — Institute for Mathematical Physics, TU Braunschweig, Germany

An adiabatic exchange of Majorana bound states reveals their exotic anyonic nature. Here we propose an experimental setup consisting of a Corbino-geometry Josephson junction on the surface of a topological insulator, in which Majorana bound states can be created and transported. By solving the Bogoliubov-de Gennes equation, we show that two spatially separated Majorana bound states at zero excitation energy appear in the junction when two flux quanta are introduced, and that their positions can be moved by changing the superconducting phase difference across the junction. These features allow us to perform the exchange operation of the Majorana bound states if we vary the phase difference adiabatically.

TT 109.2 Fri 9:45 H 0104

Topological phases in magnetic adatom-chains on top of a Rashba superconducting surface — •Andreas Heimes, Daniel Mendler, and Panagiotis Kotetes — Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, 76131 Karlsruhe

We investigate a Majorana fermion (MF) platform consisting of a chain of magnetic adatoms placed on top of a conventional superconductor with Rashba spin-orbit coupling. By identifying the classical magnetic ground state of the adatom chain, we extract a phase diagram which exhibits ferromagnetic (FM), antiferromagnetic (AFM) as well as spiral orders. We determine the parameter regime for which the FM or AFM phases dominate over the spiral and perform a topological analysis of the low-energy electronic spectrum. To this end we derive an effective model relying on Shiba bound states. We find that for both magnetic patterns, FM and AFM, the hybrid system behaves as a topological superconductor which can harbor one or even two MFs per edge. We propose directions on how to experimentally access these different MF phases.

TT 109.3 Fri 10:00 H 0104

Localization length and non-adiabaticity - braiding errors in Majorana quantum wires — •Michael Sekania[1,3], Martin Greiter[1], Ronny Thomale[1], and Peter Schmitteckert[2] — [1]Institute for Theoretical Physics and Astrophysics, Julius-Maximilian University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany — [3]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany

Majorana fermions have been attracting substantial interest in recent years. Several experimental groups have already reported tentative observation of Majorana zero modes in quantum nanowires that are proximity-coupled to a bulk superconductor. The unambiguous detection of Majorana quasi-particles, however, has so far remained elusive. One of the ultimate experimental checks for the existence of Majorana zero modes would be a braiding experiment, that reveals the non-trivial braiding statistics of the Majorana fermions. We present numerical studies of the braiding of Majorana bound states (MBS) in presence of a quasi-particle background, and show braiding errors due to non-adiabaticity – which is a realistic scenario for experiments – and due to system sizes which are comparable to the localization length of the MBS. The latter seems to be the case for certain experimental realizations reported recently. We further address the influence of finite-range interactions on the braiding process.

TT 109.4 Fri 10:15 H 0104

Fractional Josephson Effect in HgTe based Josephson Junctions — •Jonas Wiedenmann[1], Erwann Bocquillon[1], Russel Deacon[2], Simon Hartinger[1], Luis Maier[1], Christopher Ames[1], Koji Ishibashi[2], Tarucha Seigo[3], Teun Klapwijk[4], Hartmut Buhmann[1], and Laurens Molenkamp[1] — [1]EP3, Physikalisches Institut, Universität Würzburg, Würzburg, Germany — [2]Advanced Device Laboratory, RIKEN, Japan — [3]Department of Applied Physics, Univeristy of Tokyo, Tokyo, Japan — [4]Kavli Institute of Technology, Delft University of Technology, Delft, The Netherlands

3D topological insulators are a new class of material in which electronic transport is governed by topological surface states while the bulk remains insulating. Due to the helical spin polarization of the surface states, the coupling to a conventional s-wave superconductor is predicted to lead to the emergence of zero-energy bound states at the S-TI interface. These gapless zero energy states (sometimes referred to as Majorana bound states) are topologically protected against scattering and thus give rise to a 4π periodic Josephson current.

We fabricated Josephson junctions based on the three dimensional topological insulator HgTe and study its response under external rf excitation. An unconventional A.C. Josephson effect is observed which leads us to the conclusion that a 4π contribution in the Josephson current is present. In addition to the observation of an unconventional excess current, this gives robust signatures of the presence of zero-energy states.

TT 109.5 Fri 10:30 H 0104

Josephson current and Majorana bound states through 2DEG with Spin-Orbit Interaction — •Pasquale Marra[1], Roberta Citro[1,2], and Alessandro Braggio[3] — [1]SPIN-CNR, I-84084 Fisciano (Salerno), Italy — [2]Dipartimento di Fisica "E. R. Caianiello", Universitá di Salerno, I-84084 Fisciano (Salerno), Italy — [3]SPIN-CNR, Via Dodecaneso 33, I-16146 Genova, Italy

We investigate the DC Josephson current in a two dimensional electron gas (2DEG) proximized with a s-wave superconductor, in the presence of spin-orbit interaction and magnetic field. Solving the Bogoliubov-De Gennes equations in the framework of a tight-binding Hamiltonian, we calculate the Andreev bound states, the Josephson current, and the Majorana polarization as a function of phase difference between the two superconductors. We therefore investigate the conditions under which Majorana bound states are localized at the system interfaces.

15 min. break.

TT 109.6 Fri 11:00 H 0104

Thermal conductance as a probe of the non-local order parameter for a topological superconductor with gauge fluctuations — •Fabian Hassler[1], Bernard van Heck[2], Emilio Cobanera[3], and Jascha Ulrch[1] — [1]JARA Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany — [2]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — [3]Institute for Theoretical Physics, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands

We investigate the effect of quantum phase slips on a helical quantum wire coupled to a superconductor by proximity. The effective low-energy description of the wire is that of a Majorana chain minimally coupled to a dynamical *2 gauge field. Hence the wire emulates a matter-coupled gauge theory, with fermion parity playing the role of the gauged global symmetry. Quantum phase slips lift the ground state degeneracy associated with unpaired Majorana edge modes at the ends of the chain, a change that can be understood as a transition between the confined and the Higgs-mechanism regimes of the gauge theory. We identify the quantization of thermal conductance at the transition as a robust experimental feature separating the two regimes. We explain this result by establishing a relation between thermal conductance and the Fredenhagen-Marcu string order-parameter for confinement in gauge theories. Our work indicates that thermal transport could serve as a measure of non-local order parameters for emergent or simulated topological quantum order.

TT 109.7 Fri 11:15 H 0104

Topological Kondo Effect in Transport through a Superconducting Wire with Multiple Majorana End States — •Oleksiy Kashuba and Carsten Timm — Institute für Theoretische Physik, Technische Universität Dresden

We investigate a system of multiple Majorana states at the end of a topological superconducting wire coupled to a normal lead. For a minimum of three Majorana fermions at the interface, we find nontrivial renormalization physics. Interface tunneling processes can be classified in terms of spin-1/2 and spin-3/2 irreducible representations of the SU(2) group. We show that the renormalization of the tunneling amplitudes belonging to different representations is completely

different in that one type is suppressed, whereas the other is enhanced, depending on the sign of the interaction coupling. This results in distinct temperature dependencies of the tunneling current through the interface and different spin polarizations of this current.

TT 109.8 Fri 11:30 H 0104

Topological superconductivity in Rashba semiconductors without a Zeeman field — •Panagiotis Kotetes — Karlsruhe Institute of Technology

I propose new hybrid devices based on multichannel Rashba semiconductors, which harbor Majorana fermions (MFs) without a Zeeman field [1]. In contrast, magnetic fluxes, supercurrents or electric fields can be employed, yielding an enhanced device manipulability. The generic topological phase diagram exhibits features of quantum criticality and a rich interplay of phases with 0, 1 or 2 MFs per edge. The most prominent and experimentally feasible implementation, relies on the already existing platforms of InAs-2DEG on top of a Josephson junction. Appropriate design of the latter device, allows phases with 1 or 2 MFs, both detectable in zero-bias anomaly peaks with a single or double unit of conductance. The absence of the Zeeman field in these devices could be assisting for a Kondo-peak-free interpretation of the expected MF signatures.

[1] P. Kotetes, arXiv:1409.5264.

TT 109.9 Fri 11:45 H 0104

Majorana flat bands in anisotropic systems — •Daniel Mendler, Panagiotis Kotetes, and Gerd Schön — Institut für theoretische Festkörperphysik, Karlsruher Institut für Technologie

It has been recently proposed that topologically protected Majorana flat bands (MFBs) emerge in superconductors with nodal energy spectrum. In this work we introduce a new class of gapful superconductors, in which MFBs can occur due to strong anisotropy. The prototype system exhibiting this kind of behavior is the nematic $p_x + p_y$ spinless superconductor, which supports an edge MFB with controllable bandwidth. Our proposal can be for instance experimentally implemented in topological superconductors engineered from i. semiconductors with tunable spin-orbit coupling or ii. topological insulator surfaces with intrinsic magnetic order in proximity to a conventional SC. By investigating the topological properties of both setups, we show that their unique features render them feasible platforms for manipulating the Majorana fermion bandstructure and realizing MFBs.

TT 109.10 Fri 12:00 H 0104

Topological phases of interacting fermions in one-dimensional superconductor - normal metal geometry — Dganit Meidan[1,2], •Alessandro Romito[1], and Piet W. Brouwer[1] — [1]Department of Physics, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel — [2]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

One-dimensional superconductors can be in non-trivial topological phases harboring Majorana end-states, which possess non-abelian statistics. It has been recently established that in the presence of interactions the classification of topological superconducting phases can be significantly altered. Specifically, for one-dimensional superconductors possessing a time reversal symmetry (BDI class), interactions reduce the infinitely many non-interacting phases (Z topological index) to eight distinct ones (Z_8 topological index).

In this talk I will consider multi-mode superconducting wires in such BDI class when probed by an external contact, and discuss their low temperature and voltage bias transport properties. I will first show that the Andreev reflection component of the scattering matrix of the probing lead provides a topological index, r=-4, ..., 4, which distinguish the eight topological phases. The two topologically equivalent phases with r= 4,-4 support emergent many-body end states, which are identified to be a topologically protected Kondo-like resonance. The path in phase space that connects these equivalent phases crosses a non-fermi liquid fixed point where a multiple channel Kondo effect develops.

TT 110: Superconductivity: Fe-based Superconductors – Theory

Time: Friday 9:30–12:15 Location: H 2053

TT 110.1 Fri 9:30 H 2053

Mass renormalization and unconventional pairing in multiband Fe-based superconductors- a phenomenological approach — •S.-L. Drechsler[1], S. Johnston[2], D. Efremov[1], V. Grinenko[1], H. Rosner[3], and K. Kikoin[4] — [1]IFW-Dresden — [2]Inst. of Quantum Matter, University of Brit. Coulumbia, Vancouver, Canada — [3]MPI-cPfS, Dresden, — [4]Tel Aviv University, Israel

Combining DFT calculations of the density of states and plasma frequencies with experimental thermodynamic, optical, ARPES, and dHvA data taken from the literature, we estimate both the high-energy (Coulomb, Hund's rule coupling) and the low-energy (el-boson coupling) electronic mass renormalization [H(L)EMR] for typical Fe-pnictides with T_c<40 K, focusing on (K,Rb,Cs)Fe_2As_2, (Ca,Na)122, (Ba,K)122, LiFeAs, and $LaFeO_{1-x}F_xAs$ with and without As-vacancies. Using Eliashberg theory we show that these systems can NOT be described by a very strong el-boson coupling constant $\lambda \gtrsim 2$, being in conflict with the HEMR as seen by DMFT, ARPES and optics. Instead, an intermediate $s_\pm$ coupling regime is realized, mainly based on interband spin fluctuations from one predominant pair of bands. For (Ca,Na)122, there is also a non-negligible intraband el-phonon/orbital fluctuation intraband contribution. The coexistence of magnetic As-vacancies and high-T_c =28 K for $LaFeO_{1-x}F_xAs_{1-\delta}$ excludes an orbital fluctuation dominated s_{++} scenario at least for that system. In contrast, the line nodal $BaFe_2(As,P)_2$ near the quantum critical point is found as a superstrongly coupled system. The role of a pseudo-gap is briefly discussed for some of these systems.

TT 110.2 Fri 9:45 H 2053

Magnetic and orbital ordering in the iron-based superconductors: role of spin-orbit coupling — •Felix Ahn[1], Johannes Knolle[2], Rafael Fernandes[3], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany — [3]School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455, USA

We analyze the magnetic ordering in the iron-based superconductors in presence of spin-orbit coupling. Based on several tight-binding parametrizations of the 3d electron states we show how the spin-orbit coupling introduces the anisotropy of the magnetization of the striped antiferromagnetic state by lifting the degeneracy of all three components of the magnetization m_x, m_y and m_z. The orientation of the magnetic moment is determined by the contribution of the xy, xz, and yz orbitals to the electronic states near the Fermi level of the electron and hole bands and is determined by the electron filling. We find that within an itinerant approach the magnetic ordering is most favorable along the wavevector of the striped AF state. This appears to be a natural consequence of the spin-orbit coupling in the striped AF state where the ferro-orbital order of the xz and yz orbitals is only a consequence of the striped AF order. We further analyze the role of spin-orbit coupling for the C_4 magnetic structure where SDW order parameters with both wavevectors, $Q_x = (\pi, 0)$ and $Q_y = (0, \pi)$, coexist.

TT 110.3 Fri 10:00 H 2053

Superconductivity and Magnetism from First Principles — •Andreas Linscheid, Antonio Sanna, Frank Essenberger, and Eberhard K.U. Gross — Max-Planck-Institut für Mikrostrukturphysik

Magnetism has intriguing effects in superconductors. On the one hand static magnetic fields are known to suppress the superconducting state while dynamic spin-fluctuations are the probable candidate to explain the pairing in the Fe-based Superconductors.

Achieving an ab-initio description is important. First, because this allows to compute the critical field and whether a local coexistence of magnetic and superconducting phases exist. Second, the critical temperature of a material is among the predicted properties which allows to search yet unknown superconductors on a computer.

The Density Functional Theory for Superconductors (SCDFT) has

been very successful in predicting T_c of phonon mediated superconductors. We include the magnetic density into SCDFT so that the electronic Kohn-Sham system now reproduces the electronic density $n(\mathbf{r})$, the order parameter of superconductivity $\chi(\mathbf{r}, \mathbf{r}')$ and the magnetic density $\mathbf{m}(\mathbf{r})$. We derive the xc-potential and discuss some first results.

Furthermore, we discuss an effective electron interaction mediated by spin-flip processes based on the exact spin-susceptibility. We drive a xc-functional for SCDFT that includes this effective interaction and present some results.

TT 110.4 Fri 10:15 H 2053

Coherence-incoherence crossover and non-Fermi-liquid self-energy in Hund's metals - Insights into the normal state of iron pnictide superconductors from a Numerical Renormalization Group study — •Katharina M. Stadler[1], Andreas Weichselbaum[1], Jan von Delft[1], and Gabriel Kotliar[2] — [1]Faculty of Physics, Ludwig-Maximilians-Universität München — [2]Department of Physics and Astronomy, Rutgers University, NJ, USA

In 2008, the iron pnictides were discovered as a new class of strongly correlated high-temperature superconductors [1]. The normal state of these itinerant multi-band materials shows characteristic anomalous properties, which are assigned to a coherence-incoherence crossover at very low temperatures, mediated by Hund's rule coupling.

We study a N-channel Anderson impurity model with Hund's coupling and a filling of N-1, together with the corresponding Kondo model, for the cases N=2 and 3, using the full density-matrix Numerical Renormalization Group (fdmNRG) with non-abelian symmetries [2]. Our high-quality real-frequency NRG results confirm the existence of a Fermi-liquid regime at low temperatures and a non-Fermi-liquid power-law for the self-energy in the incoherent normal state. Further, we analyse the interplay of spin and orbital degrees of freedom to gain insights into the relevant energy scales of the coherence-incoherence crossover and the corresponding renormalization group flow. In addition the lattice model is investigated within DMFT employing fdmNRG as impurity solver.

[1] Takahashi et al., Nature 453 (2008).
[2] A. Weichselbaum, Ann.Phys. 327 (2012).

TT 110.5 Fri 10:30 H 2053

Pair-breaking due to orbital magnetism in iron-based superconductors — •Mareike Hoyer[1,2], Mathias S. Scheurer[1], Sergey V. Syzranov[3,1], and Jörg Schmalian[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Germany — [3]Department of Physics, University of Boulder, Boulder, Colorado, USA

We consider superconductivity in the presence of impurities in a two-band model suited for the description of iron-based superconductors. We analyze the effect of interband scattering processes on superconductivity, allowing for orbital, i. e., non-spin-magnetic time-reversal-symmetry-breaking impurities. Pair-breaking in such systems is described by a nontrivial phase in an interband-scattering matrix element. We find that the transition temperature of conventional superconductors can be suppressed due to interband scattering, whereas unconventional superconductors may be unaffected. As an example, we consider impurities associated with orbital density waves that are of interest for iron-based superconductors.

15 min. break.

TT 110.6 Fri 11:00 H 2053

Investigation of substitution effects in the 122-family of the iron superconductors via orbital based CPA — •Alexander Herbig, Rolf Heid, and Robert Eder — Institute for Solid State Physics, Karlsruhe Institute of Technology

The iron-based superconductors are a prominent example how doping can be used as a tuning parameter for the electronic properties of a complex material. A lot of theoretical and experimental effort has been put into the investigation of this class of materials over the last half decade. But until now first principle calculations on the impact of substitution on the electronic structure using supercells and more advanced methods still are rare. Also the role of doping is not fully understood. We recently developed an implementation of Blackman, Esterling and Berk's extension of the coherent potential approximation (BEB-CPA) within a pseudopotential approach using a linear combination of atomic orbitals (LCAO) basis. We present electronic structure calculations for the 122-family using this method with various species substitutions at different sites and arbitrary impurity concentrations. In particular we investigate orbitally selective effects of substitutional disorder on electronic bands near the Fermi level and the impact of substitution on the electronic density.

TT 110.7 Fri 11:15 H 2053

Inelastic Scanning Tunneling Microscopy in conventional and unconventional superconductors — •Patrik Hlobil, Jörg Schmalian, Wulf Wulfhekel, and Jasmin Jandke — Karlsruhe Institute of Technologie, Germany

Electron tunneling spectroscopy has been used extremely successful in order to verify the microscopic phonon pairing mechanism in conventional BCS superconductors using the Eliashberg theory. Nevertheless, earlier theories and experiments focused mainly on elastic tunneling processes. We present, motivated by recent experiments, a theoretical description of inelastic tunneling in STM in which an electrons tunnels from the tip into a BCS superconductor and coherently excites a phonon during the tunneling process. This additional channel enhances the measured conductivity and we show that if the superconductor is in the normal state, within some limitations, the derivative $\mathrm{d}\sigma/\mathrm{dV}$ will be proportional to the Eliashberg function $\alpha 2\mathrm{F}$. Additionally, the influence of the inelastic contributions on the tunneling spectrum in the superconducting state will be discussed. Finally, we generalize the theory to other bosonic excitations and focus on the question if inelastic tunneling could be used to unveil the electronic pairing mechanism in the iron pnictides.

TT 110.8 Fri 11:30 H 2053

Unexpected impact of magnetic disorder on multiband superconductivity — •Dmitri Efremov[1], Maxim Korshunov[2], Alexander Golubov[3], and Oleg Dolgov[4] — [1]IFW Dresden, Germany — [2]Kirensky Institute of Physics, Krasnoyarsk, Russia — [3]University of Twente, Enschede, The Netherlands — [4]Max-Planck-Institute for Solid State Physics, Stuttgart, Germany

We analyze how the magnetic disorder affects the properties of the two-band s_{++} and s_{+-} models, which are subject of hot discussions regarding iron-based superconductors and other multiband systems like MgB_2 . We show that there are several cases when the transition temperature is not fully suppressed by magnetic impurities in contrast to the Abrikosov-Gor'kov theory, but a saturation of Tc takes place in the regime of strong disorder. These cases are: (1) the purely interband impurity scattering, (2) impurity scattering purely in one of the bands, (3) the unitary scattering limit. We show that the a transition between s_{++} and s_{+-} states may occur with increasing magnetic disorder.

TT 110.9 Fri 11:45 H 2053

Anisotropic transport properties of Ba-122 compounds calculated by the Kubo-formalism — •Gerald Derondeau[1], Sebastian Wimmer[1], Diemo Ködderitzsch[1], Hubert Ebert[1], and Ján Minár[1,2] — [1]Department Chemie, Ludwig-Maximilians-Universität München, 81377 München, Germany — [2]NewTechnologies-Research Center, University of West Bohemia, Pilsen, Czech Republic

We have shown recently that the Korringa-Kohn-Rostoker-Green function (KKR-GF) method, in combination with the coherent potential approximation (CPA), indeed provides a very suitable platform to describe the impact of substitutional disorder on the electronic structure of iron pnictide superconductors. [1]

Based on this we focused on the resistivity anisotropy of Ba-122 compounds, which lately received tremendous interest. [2, 3]

We use the Kubo-formalism to calculate the longitudinal resistivity of doped Ba-122 compounds in their antiferromagnetic state within the framework of the local approximation to density-functional-theory. We are able to reproduce the unusual resistivity anomaly and investigate the transport behavior for different substitution types in $BaFe_2As_2$. The dependence of the transport properties on the type and the concentration of the dopant suggest a crucial influence of impurity scattering for the resistivity anomaly in iron pnictides.

[1] G. Derondeau *et al.*, Phys. Rev. B **90**, 184509 (2014).
[2] J.-H. Chu *et al.*, Science **329**, 824 (2010).
[3] S. Ishida *et al.*, Phys. Rev. Lett. **110**, 207001 (2013).

TT 110.10 Fri 12:00 H 2053

Transport in the spin-density-wave phase of iron pnictides — •Maxim Breitkreiz[1], Jacob Schmiedt[1], Philip M. R. Brydon[2],

and Carsten Timm[1] — [1]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany — [2]Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, USA 20742

The metallic spin-density-wave phase of iron pnictides shows characteristic and not yet understood features such as the pronounced anisotropy of the resistivity, the enhanced Hall coefficient, and magnetoresistance. We analyze the transport behavior within the linear-response theory and take into account scattering off spin fluctuations and damped magnons. Vertex corrections turn out to be very important because of strong anisotropy in the scattering rates and the reconstructed Fermi surfaces.

TT 111: Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Friday 9:30–12:15 Location: H 3005

TT 111.1 Fri 9:30 H 3005

Hybridization effects from the hydrogenation of the correlated impurity system Fe/Pt(111) — •Maria Valentyuk[1,3], A.A. Khajetoorians[1,2], M. Steinbrecher[1], T. Schlenk[1], A. Shick[4], I. Kolorenc[4], A. Lichtenstein[1], T.O. Wehling[5], R. Wiesendanger[1], and J. Wiebe[1] — [1]Department of Physics, Hamburg University, Germany — [2]Institute for Molecules and Materials, Radboud University, The Netherlands — [3]Department of Theoretical Physics and Applied Mathematics, Ural Federal University, Ekaterinburg, Russia — [4]Institute of Physics, ASCR, Na Slovance 2, Prague, Czech Republic — [5]Institute for Theoretical Physics, Bremen Center for Computational Material Science, University of Bremen, Germany

The presence of residual H_2 gas in ultra-high vacuum chambers is known to effect structural and transport properties of metallic samples. Scaling down to the level of one atomic impurity, this metal-hydrogen interaction brings new phenomena to the multi-orbital physics of d-shell metallic adatoms. Here, we show that in such a system with strong hybridization, i.e., iron adatoms on Pt(111), the hydrogenation serves as an additional complex parameter for the manipulation of the electronic interactions. We discuss the main electronic and magnetic features of the different iron-hydride complexes coupled to the Pt(111) substrate. By means of DFT calculations and by solving the multi-orbital Anderson impurity model (ED, CT-QMC) we found a significant qualitative change in the hybridization strength of different complexes and accordingly strong modifications of the correlated electronic behaviour.

TT 111.2 Fri 9:45 H 3005

Kondo temperature in the Anderson-Holstein Model with a displacement dependent hybridization. — •Andre Jovchev and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund

Molecular junctions are potential candidates for future nano-electronic devices since they exhibit interesting phenomena such as nonlinear I-V curves and hysteresis effects attributed to conformational change in the molecule. Since the tunnel coupling depends exponentially on the distance, we have studied the influence of the vibrational couplings on the Kondo temperature in the Anderson-Holstein model(AHM) with a modified hybridisation term using the numerical renormalisation group (NRG). This includes a minimal model for the coupling of molecular vibrational modes to the electronic degree of freedom augmented with a vibrational dependent tunnelling term. Our investigation has been motivated by scanning tunnelling microscope experiments where the Kondo temperature in Co and Cu complexes on metallic surfaces has been reported to be mainly independent of the applied gate voltage which is in disagreement with the standard theory of the spin 1/2 Kondo effect.

TT 111.3 Fri 10:00 H 3005

Real-time dynamics induced by quenches across the quantum critical points in gapless Fermi systems with a magnetic impurity — •Christian Kleine[1], Julian Musshoff[2], and Frithjof B. Anders[1] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany — [2]Forschungszentrum Jülich GmbH, Institute for Advanced Simulation, 52425 Jülich, Germany

The energy-dependent scattering of fermions from a localized orbital at an energy-dependent rate $\Gamma(\epsilon) \propto |\epsilon|^r$ gives rise to quantum critical points (QCPs) in the pseudo-gap single impurity Anderson model separating a local moment phase with an unscreened spin moment from a strong-coupling phase which slightly deviates from the screened phase of standard Kondo problem. Using the time-dependent numerical renormalization group (TD-NRG) approach we show that local dynamic properties always equilibrate towards a steady-state value even for quenches across the QCP but with systematic deviations from the thermal equilibrium depending on the distance to the critical coupling. Local non-equilibrium properties are presented for interaction quenches and hybridization quenches. For interaction quenches within the screened phase we find an universal function for the time-dependent local double occupancy. We trace back the discrepancy between our results and the data obtained by a time-dependent Gutzwiller variational approach to restrictions of the wave-function ansatz in the Gutzwiller theory.

TT 111.4 Fri 10:15 H 3005

Transfering spin into an extended π-orbital of a large molecule – A comparison between NRG and experiment — •Benedikt Lechtenberg[1], Thorsten Deilmann[2], Taner Esat[3], Peter Krüger[2], Christian Wagner[3], Ruslan Temirov[3], Frithjof B. Anders[1], F. Stefan Tautz[3], and Michael Rohlfing[2] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund — [2]Institut für Festkörpertheorie, WWU Münster, 48149 Münster — [3]Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich

Recently, the adsorption of single Au atoms on a PTCDA monolayer physisorbed on a Au(111) surface has been investigated by means of low temperature scanning tunneling microscopy (STM) and spectroscopy (STS). The chemical reaction between the Au atom and PTCDA leads to the formation of a radical occupied with an unpaired spin. This radical formation can be observed as an additional zero bias differential conductance peak originating from the Kondo effect. An LDA calculation has identified the participating states of the Au-PTCDA complex, and the projected density of states from quasiparticle corrections provide all necessary first principle input parameter for the numerical renormalization group (NRG) calculation.
This talk focus on the NRG calculations and their results that are in excellent agreement with experiment: the calculated Kondo temperature matches very well the experimentally measured data.

TT 111.5 Fri 10:30 H 3005

One- and two-particle impurity Green's functions obtained using worm sampling — •Markus Wallerberger[1], Patrik Gunacker[1], Emanuel Gull[2], Giorgio Sangiovanni[3], and Karsten Held[1] — [1]TU Wien, Austria — [2]University of Michigan, Ann Arbor MI, USA — [3]Universität Würzburg, Germany

The single impurity Anderson model (SIAM) is one of the fundamental models of electronic correlation and lies at the computational core of dynamical mean field theory and diagrammatic extensions thereof. A state-of-the-art method for solving the SIAM is the continuous-time quantum Monte Carlo method in its hybridisation expansion (CT-HYB), because it is free of systematic bias and thus numerically exact.

In CT-HYB, one expands the partition function in terms of the hybridisation with the bath and stochastically sums the resulting diagrammatic series. The many-body propagators are usually obtained as a "by-product" of partition function sampling, as this allows for an easy implementation. We however show that this method leads to severe ergodicity problems for strong insulators and fails to yield spin-flip and pair-hopping terms of the vertex in high-symmetry cases.

Worm sampling avoids above complications by directly sampling the many-body propagators. We show that its use in CT-HYB significantly improves the quality and statistical uncertainties of the propagators. We also demonstrate how by using worm sampling for the impurity vertex, one can calculate frequency boxes of arbitrary sizes.

15 min. break.

TT 111.6 Fri 11:00 H 3005

Correlation effects in the extended Anderson model — •David Hämmerle[1], Lukas Merker[2], Theo A. Costi[2], and Sabine Andergassen[1,3] — [1]Universität Wien — [2]Forschungszentrum Jülich — [3]Universität Tübingen

We investigate the single-impurity Anderson model with an on-site Coulomb interaction U supplemented by $U'_{L/R}$ between the dot and the leads. Using the functional renormalization group in the static approximation we compute the linear conductance and the charge and spin susceptibilities at $T = 0$. The accuracy of our results is assessed by a comparison to NRG calculations. We analyze the physical behavior resulting from the competition between the Kondo effect and the characteristic power-laws of the interacting resonant level model. We find that for increasing $U'_{L/R}$ the effective on-site repulsion is reduced leading initially to an enhancement of the Kondo temperature. For sufficiently large $U'_{L/R}$, at particle-hole symmetry the low-energy properties resemble the ones of a charge Kondo effect as obtained for an attractive Coulomb interaction, while away from particle-hole asymmetry a power-law behavior as for the interacting resonant level model is observed. For a more realistic modelling of a molecular quantum dot we include an additional local Coulomb interaction in the leads, which lead to novel signatures in the conductance line shape.

TT 111.7 Fri 11:15 H 3005

From the weak coupling regime to the Kondo crossover within the reduced density matrix framework — •Davide Mantelli and milena grifoni — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Deutschland

When an Anderson quantum impurity is coupled to non interacting leads, many different regimes are accessible. In the weak coupling regime $\Gamma \ll k_{\mathrm{B}}T, U$ (with Γ the tunnelling coupling, T the temperature and U the charging energy), Coulomb blockade and co-tunnelling phenomena are well described within a perturbative approach in Γ. However, as the thermal energy approaches the coupling one, the perturbative method breaks down. By summing up a series of charge fluctuations events to all order in Γ we managed to reach the intermediate regime ($\Gamma \simeq k_{\mathrm{B}}T$) within the so-called "Dressed Second Order" (DSO)[1]. Considering its natural extension, the "Dressed-DSO", we achieved to describe the Kondo crossover where the thermal energy is comparable to the Kondo one ($T \simeq T_{\mathrm{K}}$). In this regime, equilibrium and non equilibrium fingerprints of the Kondo physics are carefully analysed.

[1] J. Kern and M. Grifoni, Eur. Phys. J. B **86**, 384 (2013)

TT 111.8 Fri 11:30 H 3005

Friedel oscillations at the Mott transition in fermionic systems — •Banhi Chatterjee, Jan Skolimowski, and Krzysztof Byczuk — Institute of Theoretical Physics, Faculty of Physics, University of Warsaw , Warsaw,Poland

Friedel Oscillations (FO) in the Fermi liquid, Mott insulator, and at the Mott transition are studied within one and two dimensional Hubbard model. Electronic correlations are accounted for by solving the dynamical mean-field theory equations, using numerical renormalization group, for infinite homogeneous system. Next the obtained self-energy is transfered into a real-space Dyson equation with the impurity potential. The last problem is solved numerically by exact diagonalization. We observe that in the metallic phase the amplitudes of FO are damped with increasing the interactions while the period remains unchanged. FO almost disappear close to the Mott transition and completely on the insulating side. An additional bound state is observed in the spectral function at the impurity site which splits along with the sub-bands on increasing the interactions.

TT 111.9 Fri 11:45 H 3005

Kondo physics of multi-orbital Anderson models studied by distributional exact diagonalization — Sareh Motahari and •David Jacob — Max Planck Institute of Microstructure Physics

The Anderson impurity model (AIM) plays a central role in the understanding of one of the most intriguing many-body phenomena, the Kondo effect, and is at the heart of Dynamical Mean-Field Theory. But solving the AIM especially in the multi-orbital case still poses a challenge, although numerically exact solvers such as continuous time quantum Monte Carlo (CTQMC) method and the numerical renormalization group (NRG) exist. However, CTQMC produces data only on the Matsubara axis, so that numerical analytic continuation to the real axis is necessary in order to calculate dynamical quantities on the real axis which is problematic. On the other hand the NRG method is computationally too demanding to be applied to realistic systems with more than one or two impurity levels. Here, we use the novel distributional exact diagonalization (DED) [1] method in order to study Kondo physics in multi-orbital Anderson models. In DED we stochastically generate a distribution of finite Anderson models that are solved by exact diagonalization, and the self-energy is obtained from the sample average. First, we demonstrate the validity of the method by calculating the dynamical properties of the single-orbital AIM and comparing with available exact results. Then we explore different situations in multi-orbital Anderson models, in particular the underscreened, overscreened and fully screened Kondo effects.

[1] M. Granth and H. U. R. Strand, Phys. Rev. B 86, 115111 (2012).

TT 111.10 Fri 12:00 H 3005

Non-Fermi liquid behavior from dynamical effects of impurity scattering in correlated Fermi liquids — •Pramod Kumar[1] and N. S. Vidhyadhiraja[2] — [1]Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany — [2]Theoretical Sciences Unit, JNCASR, Jakkur, Bangalore, India 560094

In this work, we have investigated the effect of disorder due to chemical substitution on the dynamics and transport properties of correlated Fermi liquids. A low frequency analysis in the concentrated and dilute limits shows that the dynamical local potentials arising through disorder averaging generate a linear (in frequency) term in the scattering rate. Such non-Fermi liquid behavior (nFL) is investigated in detail for Kondo hole substitution in heavy fermions within dynamical mean field theory. We find closed form expressions for the dependence of the static and linear terms in the scattering rate on substitutional disorder and model parameters. A full numerical solution of the dynamical mean field theory equations reveals that the nFL term will show up significantly only in certain regimes, although it is present for any non-zero disorder concentration in principle. We highlight the dramatic changes that occur in the quasiparticle scattering rate in the proximity of p_c. Remarkably, we find that the nFL behavior due to dynamical effects of impurity scattering has features that are distinct from those arising through Griffiths singularities or distribution of Kondo scales. Relevance of our findings to experiments on alloyed correlated systems is pointed out.

TT 112: Correlated Electrons: (General) Theory 3

Time: Friday 9:30–12:00 Location: H 3010

TT 112.1 Fri 9:30 H 3010

A generalized perspective on non-perturbative linked cluster expansions — Kris Coester[1], Sebastian Clever[1], Frederic Herbst[1], Sylvain Capponi[2], and •Kai Phillip Schmidt[1] — [1]TU Dortmund, Dortmund, Germany — [2]Université Paul Sabatier, Toulouse, France

We identify a fundamental challenge for any non-perturbative approach based on finite clusters resulting from the reduced symmetry on graphs, most importantly the breaking of translational symmetry, when targeting the properties of excited states. A generalized notion of cluster additivity is introduced, which is used to formulate an optimized scheme of graph-based continuous unitary transformations allowing to solve and to physically understand this major issue. Most importantly, it demands to go beyond the paradigm of using the exact eigenvectors on graphs.

TT 112.2 Fri 9:45 H 3010

Plasmons in strongly correlated systems: spectral weight transfer and renormalized dispersion — •Erik van Loon[1], Hartmut Hafermann[2], Alexander Lichtenstein[3,4], Rubtsov Alexey[5,6], and Mikhail Katsnelson[1,4] — [1]Institute for Molecules and Materials, Radboud University Nijmegen, Nijmegen, The Netherlands — [2]Institut de Physique Théorique, CEA, CNRS, Gif-sur-Yvette, France — [3]Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany — [4]Department of Theoretical Physics and Applied Mathematics, Ural Federal University, Ekaterinburg, Russia — [5]Department of Physics, Moscow State University, Moscow, Russia — [6]Russian Quantum Center, Skolkovo, Russia

We study plasmons within the two-dimensional extended Hubbard model in the presence of long-range Coulomb interaction. Strong correlations are taken into account using self-consistent extended dynamical mean-field theory. The polarization operator is determined in the ladder approximation, which includes non-local dynamical vertex corrections. This is necessary to fulfill charge conservation and to describe plasmons in the correlated state. The calculated plasmon spectra are qualitatively different from those in the random-phase approximation: they exhibit a spectral density transfer and a renormalized dispersion with enhanced deviation from the canonical $\sqrt{q}$-behavior. Both features are reminiscent of interaction induced changes found in the single-electron spectra of strongly correlated systems.

TT 112.3 Fri 10:00 H 3010

Phonon spectral function from continuous-time quantum Monte Carlo — •Manuel Weber, Fakher F. Assaad, and Martin Hohenadler — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We show that the phonon spectral function of electron-phonon systems can be measured with the CT-INT quantum Monte Carlo method with the help of a generating functional. We study the evolution of the phonon spectral function across metal-insulator transitions driven by electron-phonon and electron-electron interaction in the half-filled spinless Holstein and spinful Holstein-Hubbard models, respectively. In the adiabatic regime, the phonons soften at the zone boundary on approaching the Peierls transition. In the metallic phase, we observe the hybridization of the phonon mode with the particle-hole continuum, and a pronounced transfer of spectral weight between phonon and particle-hole excitations as a function of the phonon frequency.

TT 112.4 Fri 10:15 H 3010

Magnetic properties of FeAl — •Anna Galler[1], Ciro Taranto[1], Markus Wallerberger[1], Merzuk Kaltak[2], Giorgio Sangiovanni[3], Alessandro Toschi[1], Georg Kresse[2], and Karsten Held[1] — [1]Institut für Festkörperphysik, TU Wien — [2]Department of Computational Materials Physics, Universität Wien — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg

While the intermetallic FeAl is found to be paramagnetic in experiment, standard band-theory predicts the material to be ferromagnetic. We show that this discrepancy can be overcome by a better treatment of electronic correlations within LDA+DMFT (local density approximation combined with dynamical mean field theory). In fact, our results show no magnetization and a paramagnetic Pauli-like susceptibility for the whole range of temperature investigated. The origin for this behavior are short-time local magnetic moments that fluctuate in time.

We performed bandstructure calculations and projected the low energy part of the Hamiltonian onto a set of 9 maximally localized Wannier orbitals. The interaction parameters for our $d+p$ model were computed within cRPA and for the numerical solution of the impurity problem we used a continuous-time quantum Monte Carlo algorithm in its hybridization expansion.

TT 112.5 Fri 10:30 H 3010

Separability of dynamical and non-local correlations in three dimensions — Thomas Schäfer, Alessandro Toschi, and •Jan Martin Tomczak — Institute of Solid State Physics, Vienna University of Technology, A-1040 Vienna, Austria

While second-order phase transitions always cause strong non-local fluctuations, their effect on spectral properties crucially depends on the dimensionality.

For the important case of three dimensions, we show that the electron self-energy is well separable into a local dynamical part and static non-local contributions. In particular, our non-perturbative many-body calculations for the 3D Hubbard model at different fillings demonstrate that the quasi-particle weight remains essentially momentum-independent, also in the presence of overall large non-local corrections to the self-energy.

Relying on this insight we propose a "space-time-separated" scheme for many-body perturbation theory that is up to ten times more efficient than current implementations. Besides these far-reaching implications for state-of-the-art electronic structure schemes, our analysis may also provide guidance to the quest of going beyond them.

[1] arXiv:1411.5686

15 min. break.

TT 112.6 Fri 11:00 H 3010

What is the fate of the Mott metal-insulator transition in two dimensions? — •Thomas Schäfer[1], Faruk Geles[2], Daniel Rost[3,4], Georg Rohringer[1], Enrico Arrigoni[2], Karsten Held[1], Nils Blümer[3], Markus Aichhorn[2], and Alessandro Toschi[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Institute of Theoretical and Computational Physics, Graz University of Technology, Graz, Austria — [3]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [4]Graduate School Materials Science in Mainz, Johannes Gutenberg University, Mainz, Germany

One of the most fundamental hallmarks of the physics of strong electronic correlations is, undoubtedly, the Mott-Hubbard metal-insulator transition (MIT), whose properties can be well captured in infinite dimensions. However, astonishingly little is known in the case of finite dimensions where spatial correlations become dominant. Our analysis of the two-dimensional Hubbard model on a square lattice demonstrates that at low temperatures the critical interaction for the onset of an insulator is progressively reduced towards zero by the inclusion of spatial correlations on longer and longer length scales. Eventually an insulating spectral gap is always opened at low-enough temperatures by (non-local) antiferromagnetic Slater paramagnons, so that the MIT completely disappears in this case [1].

[1] T. Schäfer, F. Geles, D. Rost, G. Rohringer, E. Arrigoni, K. Held, N. Blümer, M. Aichhorn and A. Toschi, arXiv:1405.7250

TT 112.7 Fri 11:15 H 3010

First order character and observable signatures of topological quantum phase transitions — •Adriano Amaricci[1], Jan Budich[2,3], Bjoern Trauzettel[4], Massimo Capone[1], and Giorgio Sangiovanni[4] — [1]Democritos National Simulation Center, Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali (IOM) and Scuola Internazionale Superiore di Studi Avanzati (SISSA), Via Bonomea 265, 34136 Trieste, Italy — [2]Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria — [3]Institute for Quantum Optics and Quantum Information, Austrian Academy of Sciences, 6020 Innsbruck, Austria — [4]Institut fur Theoretische Physik und Astrophysik, Universitat Wuerzburg, Am Hub-

land, D-97074 Wuerzburg, German

Topological quantum phase transitions are characterised by changes in global topological invariants beyond the paradigm of spontaneous symmetry breaking. For non-interacting electrons, such transitions are continuous and always accompanied by a gap-closing in the energy spectrum. Here, we demonstrate that sufficiently strong electron-electron interaction can fundamentally change the situation: we discover a topological quantum phase transition of first order character in the genuine thermodynamic sense, that occurs without gap closing. Our theoretical study reveals the existence of a quantum critical endpoint associated with an orbital instability on the transition line between a 2D topological insulator and a trivial band insulator. Remarkably, this phenomenon entails unambiguous signatures associated to the orbital occupations that can be detected experimentally.

TT 112.8 Fri 11:30 H 3010

Metal-insulator transitions in the Falicov-Kimball Model — •Younes Javanmard[1,2], Andrey Antipov[3], Pedro Ribeiro[4], and Stefan Kirchner[5] — [1]Max Planck Institute for Physics of Complex Systems, Nothnitzer str.38, 01187, Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Nothnitzer str. 40, 01187, Drsden, Germany — [3]Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA — [4]Russian Quantum Center, Novaya street 100A, Skolkovo Village, Odintsovo district, Moscow area, 143025 Russia — [5]Center for Correlated Matter, Zhejiang University, Hangzhou, China

How an insulator forms out of correlated metallic states is only partially understood. We study this issue in the Falicov-Kimball model, a proxy of the more complicated Hubbard model, that contains feature of an annealed disorder problem. For the half-filled Falicov-Kimball model on a square lattice one expects the formation of an insulator due to a CDW transition of the fully nested Fermi surface as temperature is lowered. In the limit of infinite interaction strength the nature of this transition is well understood. On the other hand, increasing the interaction strength at fixed temperature well above the CDW onset, the density of states at the Fermi energy vanishes. We set up a stochastic approach on finite systems that allows us to study both the evolution of the Inverse Participation Ratio and the change of the nature of the CDW transition with increasing interaction strength and system size. We discuss emergent localization within the disordered phase near the metal-insulator transitions of this model.

TT 112.9 Fri 11:45 H 3010

Analytic Continuation Using Stochastic Sampling - Efficient Sampling, Functional Reformulation and Parameter Selection — •Khaldoon Ghanem and Erik Koch — German Research School for Simulation Sciences, Jülich, Germany

The stochastic sampling method (StochS) is used for the analytic continuation of quantum Monte Carlo data from the imaginary axis to the real axis. Compared to the maximum entropy method (MaxEnt), StochS does not have explicit parameters, and it has the potential for resolving sharp features in the spectrum.

We present a new efficient algorithm for performing StochS called Blocked Mode Sampling (BMS). In comparison to earlier StochS methods, BMS reduces the computational times by orders of magnitude. We find that StochS results depend on the discretization, an effect which has not been discussed before in the literature. We show that the grid dependence implies a default model and that by reformulating the method in function space, we can make the default model explicit and get grid-independent results. Demanding proper functional Bayesian formulation of any analytic continuation method excludes MaxEnt and Tikhonov regularization. Therefore, StochS is currently the only available Bayesian method and is actually one of the simplest methods with minimal parameters. Finally, we present guidelines for choosing the default model of StochS and its grid. This gives good results in practice and can be used as a starting point for a more rigorous treatment in the future.

TT 113: Organic Electronics and Photovoltaics: Devices (jointly with CPP, HL)

Time: Friday 9:30–12:00 Location: C 130

Invited Talk TT 113.1 Fri 9:30 C 130

Strong and switchable magnetic couplings in molecular semiconductor films — •Michele Serri[1], Wei Wu[1,2], Luke Fleet[1], Cyrus Hirjibehedin[2], Nicholas Harrison[1], Chris Kay[2], Andrew Fisher[2], Gabriel Aeppli[2], and Sandrine Heutz[1] — [1]London Centre for Nanotechnology, Imperial College London, UK — [2]London Centre for Nanotechnology, University College London, UK

Polyaromatic molecular thin films are well established as alternative semiconductors, but their magnetic properties have received less attention. This presentation will focus on phthalocyanines (Pc), archetypal molecular semiconductors that can ligate spin-bearing transition metals at their centre. They can be processed as thin films and nanowires [1] from the vapour phase and crystallise as a range of polymorphs. This leads to the formation of spin chains, and may give rise to magnetic exchange whose sign and magnitude depends on the nature of the transition metal and crystal structure [2]. A recent milestone was reached by CoPc, which exhibits antiferromagnetic coupling, with an exchange energy reaching 100 K [3]. This interaction is up to two orders of magnitude larger than in other first-row transition metal Pcs and can be obtained on flexible plastic substrates.

[1] Wang et al. ACS Nano 4 (2010) 3921. [2] Heutz et al. Adv. Mater. 19 (2007) 3618. [3] Serri et al. Nat. Commun. 5 (2014) 3079.

15 min. break

TT 113.2 Fri 10:15 C 130

Effects of Coulomb repulsion on conductance switching in organic molecules — •Irina Petreska[1,2] and Gertrud Zwicknagl[1] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, 38 106 Braunschweig, Germany — [2]Faculty of Natural Sciences and Mathematics, Ss. Cyril and Methodius University, 1 000 Skopje, Republic of Macedonia

Charge transfer in phenylene ethynylene oligomers (OPEs), using realistically estimated effective model parameters from first principles is studied by a combined, ab initio and model approach. The aim of our work is to investigate the Coulomb correlation effects on conductance switching in OPEs. In the proposed model, molecular electronic system is restricted to one-level coupled to metallic leads, described by a two-site Hubbard Hamiltonian. Comparison of the current-voltage curves, obtained from rate equations, for the planar and perpendicular conformer, clearly demonstrates enhancement of the switching process due to two-particle correlations.

TT 113.3 Fri 10:30 C 130

Enhanced performance of polymeric electron injection layers for OLEDs by the use of a solvent-additive. — •Sebastian Stolz[1,5], Martin Petzoldt[2,5], Naresh Kotadiya[1,5], Eric Mankel[3,5], Manuel Hamburger[2,5], Uli Lemmer[1,4], Norman Mechau[1,5], and Gerardo Hernandez-Sosa[1,5] — [1]Karlsruhe Institute of Technology, Light Technology Institute — [2]University of Heidelberg, Institute of Organic Chemistry — [3]Technische Universität Darmstadt, Materials Science Institute, Surface Science Division — [4]Karlsruhe Institute of Technology, Institute of Microstructure Technology — [5]InnovationLab GmbH, Heidelberg

In this work, we investigate an amino-functionalized polyfluorene as electron injection layer in OLEDs. We demonstrate that its performance can be considerably increased by adding a functionalized alkane to the polyfluorene solution. X-ray photoelectron spectroscopy shows that the polymer thickness decreases with increasing additive concentration which indicates a better packing of the polymers. At the same time, Ultraviolet photoelectron spectroscopy reveals that the cathode work-function decreases with increasing additive concentration. Finally, we solution process OLEDs that use a PPV derivative commonly known as Super-Yellow as emitting layer and the polyfluorene in combination with silver as cathode layer. OLEDs, that use a mixture of functionalized alkane and polyfluorene, exhibit an about 0.8 eV lower turn-on voltage while the maximum luminance is almost doubled compared to OLEDs without additive. Furthermore, operational lifetimes are improved by a factor of two.

TT 113.4 Fri 10:45 C 130

Modeling of organic semiconductors: from molecular to device properties — Pascal Kordt[1], Mustapha Al Helwi[2,3], Wolfgang Kowalsky[3], Falk May[4], Alexander Badinski[5], Christian Lennartz[4], and •Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]BASF SE, GVE/M-B009, 67056 Ludwigshafen, Germany — [3]IHF Institut, Technische Universität Braunschweig, Brunswick, Germany — [4]BASF SE, GVE/M-B009, 67056 Ludwigshafen, Germany — [5]BASF SE, GVM/S-B009, 67056 Ludwigshafen, Germany

We review the progress in modeling of charge transport in disordered organic semiconductors on various length-scales, from atomistic to macroscopic. This includes evaluation of charge transfer rates from first principles, parametrization of coarse-grained lattice and off-lattice models, and solving the master and drift-diffusion equations. Special attention is paid to linking the length-scales and improving the efficiency of the methods. All techniques are illustrated on an amorphous organic semiconductor, DPBIC, a hole conductor and electron blocker used in state of the art organic light emitting diodes (OLEDs). The outlined multiscale scheme can be used to predict OLED properties without fitting parameters, starting from chemical structures of compounds.

TT 113.5 Fri 11:00 C 130

Combined electrical and optical analysis of the efficiency roll-off in phosphorescent organic light-emitting diodes — Sebastian Wehrmeister[1], •Tobias D. Schmidt[1], Lars Jäger[1], Thomas Wehlus[2], Andreas F. Rausch[2], Thilo C. G. Reusch[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, 86153 Augsburg — [2]OSRAM OLED GmbH, 93049 Regensburg

We present a method for a comprehensive analysis of the efficiency roll-off with current density in phosphorescent organic light-emitting diodes (OLEDs). By combining electrical and optical excitation in time-resolved spectroscopic experiments we are able to measure the excited states lifetime for different driving conditions. It is thus possible to correlate changes of the triplet lifetime with a decrease of the radiative quantum efficiency of the emitting system due to exciton quenching processes. As compared to the conventional analysis of the measured external quantum efficiency (EQE) in dependence of the applied current density, the lifetime analysis is not affected by changes of the charge carrier balance with current, which can have a significant impact on the interpretation of the results. With this method we show that triplet-polaron quenching is the dominating quenching mechanism for the red phosphorescent emitter $Ir(MDQ)_2(acac)$ doped into an α-NPD matrix up to current densities of $100\,mA/cm^2$.

TT 113.6 Fri 11:15 C 130

Influence of Molecular Orientation on the Coupling of Excitons to Surface Plasmons in Semitransparent Inverted Organic Solar Cells — •Mark Gruber, Michael Mayr, Björn Gallheber, and Wolfgang Brütting — Institute for Physics, University of Augsburg, Germany

To prove the principle of coupling between surface plasmons (SPs) and excitons, we investigated semi-transparent organic solar cells, in which SPs are excited at interfaces of thin metal films and a dielectric medium by using a Kretschmann configuration setup. Therefore it is essential, that the dielectric medium has a smaller refractive index than glass, e.g. LiF or air.

To compare the SP coupling to different orientations of the transition dipole moment, two donor materials were used, diindenoperylene (DIP) and dibenzo-tetraphenyl-periflanthen (DBP). Both molecules have the transition dipole moment along the long axis. While DIP crystallizes with nearly upright standing molecules on the underlying PCBM film, DBP grows amorphous with predominantly lying molecules.[1,2] To locate the angular position of the SP resonance the reflectance of the OPVC is measured angle dependent. A simultaneously measured photo current reveals the impact of SPs in these OPVCs. The use of different donors shows, that coupling from SPs to excitons only leads to a positive effect for upright-standing transition dipole moment orientation.

[1] Wagner et al., Adv. Func. Mater. **20**, 4295, 2010.
[2] Grob et al., Appl. Phys. Lett. **104**, 213304, 2014.

Invited Talk TT 113.7 Fri 11:30 C 130

Excitonic phenomena in molecular semiconductors — •Jens Pflaum — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ZAE Bayern, 97074 Würzburg

Excitons constitute the primary electron-hole excitation in organic solid states and offer a broad range of photo-physical phenomena. In this talk we will address two key aspects of excitonic states in molecular semiconductors: i) their sensitivity to structural ordering on various length scales and ii) their implementation as recombination sites yielding access to microscopic current characteristics.

In case of i), we will discuss the impact of molecular packing on the exciton motion [1] and how long-range exciton diffusion enables access to boundary-induced trap states that might lead to suppression of otherwise prominent singlet exciton decay channels [2]. Regarding ii), the non-invasive optical read-out of molecular recombination dynamics will be demonstrated to provide information on the local current density [3]. As a consequence, by utilizing the triplet emission of suited molecules this approach paves the way towards electrically driven single photon sources operating at room temperature [4]. Financial support within the DFG research programme SPP1355 and FOR1809 is acknowledged.

[1] A. K. Topczak, et al., Phys. Rev. B 89, 201203(R) (2014).
[2] B. Gieseking, et al., Phys. Rev. B 90, 205305 (2014).
[3] B. Stender, et al., Adv. Mater. 25, 2943 (2013).
[4] M. Nothaft, et al., Nature Comm. 3, 628 (2012).

TT 114: Transport: Molecular Electronics (jointly with CPP, HL, MA, O)

Time: Friday 9:30–12:15 Location: H 0110

TT 114.1 Fri 9:30 H 0110

Phononic and thermoelectric properties of π-stacked molecular junctions — •Thomas Hellmuth[1,3], Marius Bürkle[2], and Fabian Pauly[1] — [1]Theorie der Nanostrukturen, Universität Konstanz, 78457 Konstanz, Germany — [2]Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology, Japan — [3]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76131 Karlsruhe,Germany

We present our newly developed approach to compute phonon thermal transport through nanosystems from first principles using density functional theory combined with non-equilibrium Green's function techniques. Combining both electron and phonon transport, we analyze the heat transport and thermoelectric properties of π-stacked paracyclophane molecules contacted to gold electrodes [1]. We show that, depending on temperature, the phononic contribution to the heat conductance is a factor of about 5 larger than the electronic one. By calculating the thermoelectric coefficients in linear response, we estimate the figure of merit ZT of the single-molecule junctions for different molecular lengths and substituents.

[1] M. Bürkle, T. J. Hellmuth, F. Pauly, Y. Asai, submitted.

TT 114.2 Fri 9:45 H 0110

Conductance and thermopower of C_{82} and endohedral metallofullerene molecular junctions with Au electrodes — •Marius Buerkle[1], See Kei Lee[2], Ryo Yamada[2], Hirokazu Tada[2], and Yoshihiro Asai[1] — [1]AIST, NRI, Tsukuba, Japan — [2]Graduate School of Engineering Science, Osaka University, Japan

By combining STM based conductance and thermopower measurements with first-principle transport calculations we investigate the thermoelectric properties of single C_{82} molecules, and its endohedral metallofullerene (EMF) derivatives $Gd@C_{82}$ and $Ce@C_{82}$ bridging Au electrodes. All three molecular junctions show a comparable conductance of around 0.2 G0 and a negative thermopower indicating electron-like transport through the lowest unoccupied molecular orbital (LUMO). However, for the EMF junctions a much larger thermopower is observed which we can relate to changes in the electronic structure induced by the lanthanide atoms.

TT 114.3 Fri 10:00 H 0110

A scaling relation in the vibronic contribution to the current noise — •Yoshihiro Asai — AIST, Tsukuba, Japan

The electron-phonon coupling effect on the electric current noise is studied based on the fully self-consistent theory of electron and phonon currents (SCEPC) given in terms of the Keldysh Greens function method [1], which has been successful in describing the local heating phenomena [2] and the temperature dependence of the electric conductance [3,4]. Based on the theoretical result on the noise accompanying the vibronic current, we will discuss a scaling relation between the two quantities derived from the current noise and the electric conductance at finite bias voltage. We found that the scaling relation holds when the dynamics of the electron satisfies a specific condition. We will describe these in the talk.

[1] Y. Asai, Phys. Rev. B 78, 045434-1-24 (2008).
[2] Y. Asai, Phys. Rev. B, 84, 085436-1-7 (2011).
[3] S.-K. Lee, R. Yamada, S.Tanaka, G.-S. Chang, Y. Asai, and H. Tada, ACS Nano, 6, 5078-5082 (2012).
[4] Y. Asai, Phys. Rev. B 86, 201405(R)-1-4 (2012).

TT 114.4 Fri 10:15 H 0110

Thermo-voltage of nano-thermocouples — •Ayelet Ofarim, Bastian Kopp, Johannes Boneberg, Paul Leiderer, and Elke Scheer — University of Konstanz, Department of Physics, Konstanz, Germany

As the down-scaling of electronic components continues, engineering the devices has become a challenge, in particular in view of energy and heat management. Study of thermoelectric effects in nanostructures gives important additional information about charge transport, also regarding possible life-time limiting phenomena and applications for the conversion of light energy via heat into electrical energy. The scope of this presentation is to gain deep insight into the charge transport mechanism, by studying thermo-voltage effects of metallic atomic-sized contacts [1]. We present the concept for determination of the thermo-voltage of nano-thermocouples, using a novel mechanically-controlled break junction (MCBJ) mechanism. A technique to create and detect a temperature gradient, using laser irradiation, is also presented.

[1] B. Kopp, Z. Yi, D. Benner, F. Q. Xie, C. Obermair, T. Schimmel, J. Bonenberg, P. Leiderer and E. Scheer, Beilstein J. Nanotechnol. 3, 703 (2012).

TT 114.5 Fri 10:30 H 0110

Quantum interference in thermoelectric molecular junctions: A toy model perspective — •Daijiro Nozaki[1], Stas. M. Avdoshenko[2], Haldun Sevinçli[3], and Gianaurelio Cuniberti[1,4,5] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Department of Chemistry and Institute for Computational Engineering and Sciences, University of Texas at Austin, USA — [3]Department of Materials Science and Engineering, Izmir Institute of Technology, Turkey — [4]Dresden Center for Computational Materials Science (DCCMS), TU Dresden, Germany — [5]Center for Advancing Electronics Dresden (cfAED), TU Dresden, Germany

In order to reveal the relationship between the line shape of the transmission spectra affected by quantum interference and the electronic structures, we consider a homogeneous toy model where all on-site energies are identical and model four types of molecular junctions due to their topological connectivities. We systematically analyze their transmission spectra, density of states, and thermoelectric properties. Even without the degree of freedom for on-site energies an asymmetric Fano peak could be realized in the homogeneous systems with the cyclic configuration. We also calculate the thermoelectric properties of the model systems with and without fluctuation of on-site energies. Even under the fluctuation of the on-site energies, the finite thermoelectrics are preserved for the Fano resonance, thus cyclic configuration is promising for thermoelectric applications.

[1] D. Nozaki, H. Sevinçli, S. M. Avdoshenko, G. Cuniberti, J. Appl. Phys. 117, 074308 (2014).

TT 114.6 Fri 10:45 H 0110

Effect of nonadiabatic electronic-vibrational interactions on the transport properties of single-molecule junctions — •André Erpenbeck[1], Rainer Härtle[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik und Interdisziplinäres Zentrum für Molekulare Materialien (ICMM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]nstitut für theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

The interaction between electronic and vibrational degrees of freedom in single-molecule junctions may result from the dependence of the electronic energies or the electronic states of the molecular bridge on the nuclear displacement. The latter mechanism leads to a direct coupling between different electronic states and is referred to as nonadiabatic electronic-vibrational coupling. Employing nonequilibrium Green's functions in combination with the self-consistent Born approximation, we study the influence of nonadiabatic electronic-vibrational coupling in model molecular junctions. Thereby we distinguish between systems with well separated and quasi-degenerate electronic levels. Our results show that the nonadiabatic electronic-vibrational interaction can have a significant influence on the transport properties [1]. The underlying mechanisms are analyzed with respect to the different signatures of nonadiabatic and adiabatic electronic-vibrational coupling, the relevant transport channels, negative differential resistance and quantum interference effects.

[1] A. Erpenbeck et. al., arXiv:1411.5844 (2014)

15 min. break.

TT 114.7 Fri 11:15 H 0110

Significant role of end groups in electrical transport through molecules — •Karthiga Kanthasamy[1], Markus Ring[2], Fabian Pauly[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität, Hannover, Germany — [2]Fachbereich Physik, Universität Konstanz, Germany

Mechanically controllable break junction (MCBJ) technique is used to investigate the electronic properties of ferrocene and phenyl based molecules with different end groups. Stepwise changes in conductance are observed below 1Go after insertion of the molecules. The junctions are opened in vacuum and IV curves are measured for various distances between the electrodes. Detailed analysis of IV curves shows characteristic peaks in the first-order derivative for ferrocene dithiol (FDT) molecules, which are absent in ferrocene diamine (FDA) and biphenyl dithiol (BPDT). For FDT, in the range of 0.56Go to 0.09Go, there are two symmetric peaks, whose energy difference increases from 60 meV to 160 meV with increasing contact distance. Above 0.56Go or below 0.01Go, symmetric peaks are absent. The FDT molecules show typically a one order of magnitude higher conductance than FDA and BPDT. The IV graph for FDT is linear, i.e., it has metallic characteristics, while FDA and BPDT are dominated by tunneling. Theoretical calculations for the molecules in different configurations between the gold electrodes are performed based on density functional theory and the non-equilibrium Green's function formalism. Both elastic transport properties and inelastic electron tunneling spectra are studied to explain the experimental observations.

TT 114.8 Fri 11:30 H 0110

Photoinduced transient current through a molecular junction: Effects of lead excitation — •Yaroslav Zelinskyy[1,2], Yoram Selzer[3], and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [2]Bogolubov Institute for Theoretical Physics, National Academy of Science of Ukraine, 14-b Metrologichna str., UA-03683, Kiev, Ukraine — [3]School of Chemistry, Tel Aviv University, Ramat Aviv, 69978 Tel Aviv, Israel

Laser pulse induced transient currents through a molecular junction are studied in the framework of a density matrix theory. By focusing on the sequential transport regime two types of lead excitation are considered. Firstly, effects of collective plasmon excitations of the leads and their resonant coupling to molecular excitations are investigated. If such a resonant coupling cannot be realized a second excitation regime would be of interest. Now, the nonequilibrium dynamics of individual lead electrons affect the transient current formation. While a resonant coupling to lead plasmon excitations induces a remarkable current enhancement nonequilibrium electron distributions in the leads determine the transient current mainly by their thermalization process. The theoretical framework described above is used to analyze time-resolved conductance measurements of molecular junctions based on Ferrocene molecules.

[1] L. Wang and V. May, Phys.Chem.Chem.Phys. 13, 8755 (2011).
[2] Y. Zelinskyy and V. May, Nano Lett. 12, 446 (2012).
[3] Y. Zelinskyy, Y. Selzer and V. May, Phys. Rev. B (submitted)).

TT 114.9 Fri 11:45 H 0110

***Ab-initio* model of extended CNT-metal contact** — Artem Fediai[1,2,3], •Dmitry Ryndyk[1,2,3], and Gianaurelio Cuniberti[1,2,3]

— [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [3]Dresden Center for Computational Materials Science (DCCMS), TU Dresden, 01062 Dresden, Germany

Relevant CNT-metal contacts belong to so-called extended type. Current flows from electrodes into CNT in a distributed manner, and contact resistance depends on the contact length. In such circumstances the standard *ab-initio* based transport techniques to calculate electron transport should be modified.

We have developed a special method which allows calculation of transport in the systems with metal-CNT contacts at *ab-initio* level. It takes into account both internal and external parts of the CNT-metal contact and requires simulation of the one principal and two auxiliary atomistic systems. Results of *ab-initio* calculations are then subjected to special treatment and being used in Green function formalism afterwards.

This method was applied to Al-CNT and Pd-CNT extended contacts. Results agree perfectly with existing experimental data being indeed obtained at a purely *ab-initio* level.

TT 114.10 Fri 12:00 H 0110

Hierarchical Quantum Master Equation Approach to Vibrationally Coupled Electron Transport in Single-Molecule Junctions — •Christian Schinabeck[1], Rainer Härtle[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

We investigate vibrationally coupled transport in single-molecule junctions using the hierarchical quantum master equation (HQME) approach [1-3]. This method allows a systematic convergence of the reduced dynamics of open quantum systems beyond the traditional Markovian rate equations. Within the HQME framework, two different approaches are presented and compared, which describe the vibrational degrees of freedom as part of the system or the bath, respectively. The methodology is applied to a model molecular junction consisting of a molecular level coupled to fermionic leads as well as a vibrational mode. For this system, the accurate results of the hierarchical quantum master equation approach are compared with Markovian rate equation as well as fourth-order time-nonlocal master equation calculations in different parameter regimes. The convergence properties of the two HQME approaches are analyzed in detail.

[1] Y. Tanimura *et al.*, J. Phys. Soc. Jpn. 75, 082001 (2006).
[2] F. Jiang *et al.*, Phys. Rev. B 85, 245427 (2012).
[3] R. Härtle *et al.*, Phys. Rev. B 88, 235426 (2013).

TT 115: Metallic Nanowires on the Atomic Scale (jointly with DS, O)

Time: Friday 9:30–13:15 Location: H 2032

Invited Talk TT 115.1 Fri 9:30 H 2032

From 2D to 1D: Honeycomb crystals and their nanoribbons — •Friedhelm Bechstedt — Friedrich-Schiller-Universitaet Jena, Germany

Metal-induced quantum wires are usually prepared on Si and Ge surfaces. Novel two-dimensional (2D) sheet crystals silicene, germanene and stanene as well as their functionalized counterparts are prototypes to study such atomically-thin layer systems.

Their exotic properties are studied using modern electronic-structure methods and discussed in the light of available experiments:

(i) Despite partial sp^3-bonding Dirac cones appear in their band structure similar to the sp^2-bonded graphene.

(ii) The infrared absorbance is given by the Sommerfeld fine-structure constant.

(iii) Chemical functionalization opens significant fundamental gaps. Excitons occur with giant binding energies.

(iv) A quantum spin Hall phase is due to spin-orbit interaction.

According to recent predictions one-dimensional structures, i.e., nanoribbons, should conduct electricity with 100% efficiency at room temperature with zero resistance along their edges. The predictions are critically discussed. The influence of magnetic ordering of edge states and external electric fields are investigated.

TT 115.2 Fri 10:00 H 2032

Impurity-mediated early condensation of an atomic layer electronic crystal: oxygen-adsorbed In/Si(111)-(4x1)/(8x2) — •Stefan Wippermann[1], Wolf Gero Schmidt[2], Deok Mahn Oh[3], and Han Woong Yeom[3] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — [2]Universität Paderborn, D-33098 Paderborn, Germany — [3]Pohang University of Science and Technology, Pohang 790-784, Korea

While impurities have been widely known to affect phase transitions, the atomistic mechanisms have rarely been elucidated. The self-assembled In/Si(111)-(4x1) nanowire array is an extremely popular model system for one-dimensional electronic systems and features a reversible temperature-induced phase transition into a charge density wave (CDW) ordered state, a representative electronic phase.

We present a joint experimental and *first principles* study, demonstrating oxygen impurity atoms to condense the In/Si(111) nanowire array locally into its CDW ordered ground state, even above the transition temperature. Interestingly, CDW ordering is not induced by single impurities, but instead by the cooperation of multiple impurities. The mechanism is explained as a coherent superposition of the local impurity-induced lattice strain, stressing the coupled electronic and lattice degrees of freedom for CDW ordered phases.

TT 115.3 Fri 10:15 H 2032

Transport in spatially confined anisotropic systems — •Frederik Edler[1], Ilio Miccoli[1,2], Herbert Pfnür[1], and Christoph Tegenkamp[1] — [1]Institut für Festkörperphysik, Univ. Hannover, DE — [2]Dept. Innovation Engineering, Univ. Salento, IT

Atomic chain ensembles are 1D-prototype systems with intriguing electronic properties, e.g. Peierls driven metal-insulator transitions (MIT). While such inherent instabilities can be probed smartly by surface transport, details of the phase transitions depend crucially on atomic-sized imperfections. In order to correlate such imperfections (including finite size effects) with transport properties, a spatial constriction of the electron paths is mandatory, e.g by using appropriately designed templates.

The In/Si(111) system reveals a strong anisotropy and has been comprehensively studied of the last years. We used it here as a benchmark system to investigate systematically the effects of confinement as well as of different contact geometries which is finally important to deduce correctly the resistivity components from resistance measurements. While spatial constrictions were achieved using Si(111)-mesas structures, various 4-point probe geometries could be realized by means of a 4-tip STM/SEM system. The anisotropy of the In-4×1 has been quantified by rotating the tips gradually in squared configuration. Indeed, the sensitivity was increased by one order of magnitude by performing the transport experiments on confined areas. Furthermore, first studies of the MIT tuned by adsorption of, e.g. oxygen, have been performed and will be discussed.

TT 115.4 Fri 10:30 H 2032

Ultrafast dynamics of (quasi-1D) Pb overlayers grown on flat and vicinal Si(111) — •Abdul Samad Syed[1], Vesna Mikšić Trontl[1], Manuel Ligges[1], Mathias Sandhofer[1], Ishita Agarwal[1], Isabella Avigo[1], Daniel Lükermann[2], Christoph Tegenkamp[2], Herbert Pfnür[2], and Uwe Bovensiepen[1] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Institut für Festkörperphysik, Leibniz Universität Hannover

Due to real space anisotropy of the vicinal Si(111) surfaces, hot electrons can be expected to exhibit different dynamics along and perpendicular to the steps [1] as compare to the Si(111) flat surface. We made a comparative study of Pb overlayer structures grown on vicinal Si (557) and flat Si (111) using femtosecond time- and angle-resolved two-photon photoemission. We mapped the unoccupied electronic band structure near Γ and find that both systems have two unoccupied states at $E-E_F$=3.3 and 3.5 eV. In pump-probe experiments combined with a position sensitive electron time of flight spectrometer we analyze the ultrafast momentum dependent electron dynamics

along two in plane directions. On vicinal surfaces we observe a specific, momentum dependent population dynamics which are absent on the flat surface. This signature shows a delay in population build up of 5 fs as a function of angle with respect to the terrace direction. We assign this behavior to step-induced scattering. We gratefully acknowledge funding by the DFG through FOR1700.

[1] Roth et al., Phys. Rev. Lett. 88, 096802 (2002)

TT 115.5 Fri 10:45 H 2032

Observation of correlated spin-orbit order in a strongly anisotropic quantum wire system — •Christian Brand[1], Monika Jäger[1], Herbert Pfnür[1], Gabriel Landolt[2,3], Hugo Dil[2,4], Stefan Muff[2,4], Tanmoy Das[5], and Christoph Tegenkamp[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland — [3]Physik-Institut, Universität Zürich, Switzerland — [4]Institute of Condensed Matter Physics, École Polytechnique Fédérale de Lausanne, Switzerland — [5]Theoretical Division, Los Alamos National Laboratory, USA

The surface of 1.31 ML Pb on Si(557) reveals a highly anisotropic wire ensemble structure becoming insulating in the direction across the wires when cooling below 78 K (2D/1D transition) as seen by surface transport. The delicate interplay between the superlattice structure, band filling, and extremely large Rashba type spin-orbit interaction results in a highly correlated entangled spin- and charge-state. The spin texture close to the Fermi surface is found to be alternating and equidistant, thus Fermi nesting occurs in between bands with the opposite helicity. Furthermore, the interwire coupling has been gradually changed by adsorption of excess Pb nucleating preferentially at the step edges. The analysis of spin-resolved momentum distribution curves shows that Fermi nesting is preserved up to 0.2 ML. Both the spin-dephasing seen in ARPES as well as the increase of the spin-orbit scattering rates from former magneto transport measurements is quantitatively explained in the framework of a spin-orbit density wave.

TT 115.6 Fri 11:00 H 2032

Tuning the Playground for Spin-Polarization in Au-Induced Atom Chains on High-Index Silicon Surfaces — •Julian Aulbach[1], Joerg Schaefer[1], Steven C. Erwin[2], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg, Germany — [2]Naval Research Laboratory, Washington DC, USA

Atomic wires on semiconductor substrates allow direct access to spectroscopic studies of the low-temperature ground state of quasi-one-dimensional systems, such as a charge density wave or a Tomonaga-Luttinger liquid. A particularly intriguing concept is the use of high-index silicon surfaces of the type Si(hhk), providing tunability with respect to terrace width and adatom coverage. As a specific representative, stabilization of the Si(553) surface by Au adsorption results in two different atomically defined chain types, one made of Au atoms and one of Si. The latter, situated at the step edges, forms a honeycomb nanoribbon. At low temperature these silicene-like ribbons develop a period tripling, previously attributed to a Peierls instability. Here we report evidence from scanning tunneling microscopy that rules out this interpretation [1]. On the contrary, our results are in excellent agreement with density functional calculations [2], which reveal an antiferromagnetic ordered state, where every third Si atom at the step edge hosts a single electron [1]. Additionally we will also address the consequences for this spin ordering by varying the high index substrate.

[1] J. Aulbach et al., Phys. Rev. Lett. 111, 137203 (2013).
[2] S. C. Erwin and F. J. Himpsel, Nature Commun. 1, 58 (2010).

TT 115.7 Fri 11:15 H 2032

Vibrational properties and optical anisotropy of lead nanowires on Si(557) — •Eugen Speiser[1], Arne Baumann[1], Sandhya Chandola[1], Jochen Räthel[1], Daniel Lükermann[2], Christoph Tegekamp[2], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e. V., Department Berlin, Schwarzschildstrasse 8, 12489 Berlin, Germany — [2]Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover, Leibniz Universität Hannover, Germany

We use Raman spectroscopy and Reflectance Anisotropy Spectroscopy (RAS) to investigate the vibrational properties and anisotropic optical response of Pb nanowires on Si(557). This model system, which shows quasi-1D conductance below 78 K, consists of 1.31 ML of Pb on the Si(557) surface. The adsorption of Pb induces a refacetting of the surface into evenly stepped (223) facets, decorated by one Pb nanowire each. Above 78 K the 2D coupling between the individual wires increases and allows conductivity perpendicular to them. RAS measurements of the Si(557) surface before and after Pb deposition show that the adsorption of Pb clearly induces a reorganization of the surface. Both phases exhibit a strongly anisotropic optical conductance behavior and anisotropic optical transitions which can be associated with the Pb induced reformation of the surface. The Raman spectra show surface vibrational modes which are only present after Pb deposition. With theoretical calculations it is possible to elucidate the relation of the surface vibrational modes with atomic structure and propose structural models for the high and low temperature phases.

15 min. break.

TT 115.8 Fri 11:45 H 2032

Doping Induced 1D Plasmons in Ag Monolayer Stripes on Si(557) — •Timo Lichtenstein, Ulrich Krieg, Christoph Tegenkamp, and Herbert Pfnür — Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany

We demonstrate here by testing the plasmonic properties for the system Ag/Si(557) that the interaction between adsorbate layers of transition metal atoms and strongly anisotropic surfaces can lead to various quasi-1D signatures, which, however, are not all necessarily metallic. Using low energy electron diffraction in combination with scanning tunneling microscopy and electron energy loss spectroscopy, we correlate the structure with the properties of low dimensional collective excitations, as measured with momentum and energy resolving electron loss spectroscopy. Semiconducting structures with double periodicity along the chains are formed for Ag coverages below 0.3 ML. At higher coverages, coupled with the onset of $\sqrt{3} \times \sqrt{3}$ order, metallic wires are formed. This is evident from the appearance of plasmonic losses, which show 1D dispersion only along the wires. This 1D property even persists up to 1 ML, where a densely packed array of metallic $\sqrt{3} \times \sqrt{3}$ stripes is formed. We show evidence that the metallic property is induced by an extrinsic doping process of excess Ag atoms localized at the step edges, which can be reversibly removed and added. With this system we were able to explicitly show that the 1D plasmon frequency depends on the electron density proportional to $\sqrt{n_e}$ also in the 1D case, and that the confinement of the electrons on the wires is also dependent on doping concentration.

TT 115.9 Fri 12:00 H 2032

Optical and electronic properties of quasi-1D gold nanowires on Si(553) surfaces — •Sandhya Chandola[1], Eugen Speiser[1], Conor Hogan[2], Svetlana Suchkova[1], Jochen Räthel[1], Julian Plaickner[1], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Schwarzschildstrasse 8, 12489 Berlin, Germany — [2]Institute for Structure of Matter, CNR-ISM, Via Fosso del Cavaliere, 00133 Rome, Italy

The structures of many 1D metallic nanowire systems have not yet been sufficiently clarified, such as gold nanowires on vicinal Si surfaces. Such structures are intrinsically anisotropic and can be investigated by Reflection anisotropy spectroscopy (RAS) which is a powerful optical technique for probing electronic states of surfaces. The optical response of the Si(553)-Au and hydrogenated Si(553)-Au surfaces are measured with RAS and compared with density functional theory simulations. Good agreement between experiment and theory is obtained. Local structural elements such as the Si honeycomb chains and the gold atomic wires, yield distinctive features in the optical spectra. By comparing the optical response of the freshly prepared and hydrogenated Si(553)-Au surfaces, the spectral features can be directly attributed to particular structural elements on the surface. This combination of experiment and theory is very useful in identifying specific structural sites on the surface, which generate distinctive features in the optical response. The surface will be used to attach molecules such as 3,4-toluenedithiol. The ordered array of the molecules could act as a template for further functionalization.

TT 115.10 Fri 12:15 H 2032

Vibrational properties of Au nanowires on Si(553) and Si(111) surfaces — •Sergej Neufeld[1], Simone Sanna[1], Jochen Räthel[2], Norbert Esser[2], and Wolf-Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Physik, Universität Paderborn — [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Berlin

Metallic nanowires on semiconducting substrates such as silicon and

germanium have been attracting considerable interest in the last decade. Besides various potential applications as non ohmic conductors, they are candidate systems for the demonstration of the basic concepts of one-dimensional physics such as electron correlation and Luttinger liquid behavior. In particular, the phase transitions observed on these systems have been controversially discussed and are still poorly understood. Self organizing gold chains at vicinal surfaces such as the Si(553) and Si(111) are of particular interest, as the use of stepped templates allows to vary the geometric parameters and, thus, tune the inter-chain coupling. While well-established microscopic structural models of Au nanowires on various Si surfaces based on density functional theory are available in the literature, few is known about their vibrational properties. In this work, the phonon eigenmodes and eigenfrequencies of the Au/Si(553) and Au/Si(111) wires are calculated from first-principles at the center of the Brillouin zone. Several surface localized phonon modes are found, whose phonon frequencies can be directly compared with the spectra obtained by Raman measurements. Raman scattering efficiences are calculated in order to facilitate the comparison between experiment and theory.

TT 115.11 Fri 12:30 H 2032

Plasmonic excitations in Au/Si(553) and Au/Si(775) — •Timo Lichtenstein[1], Julian Aulbach[2], Jörg Schäfer[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg, 97074 Würzburg, Germany

Si(553) and Si(775) surfaces are highly stabilized by Au adsorption resulting in chain reconstructions of Au and Si atoms. For low temperatures the chains develop a change in periodicity not because of a Peierl's transition but because of frozen spin-polarization. Therefore, they remain metallic at low temperature. Here we study the metallicity of these systems by investigating the plasmons of the spin-split bands.

The sample quality was controlled with SPA-LEED. The plasmon dispersion was then investigated via a combination of EELS and SPA-LEED setup providing both high energy and momentum resolution. Measurements were carried out at room temperature and at 77 K.

Similar to Au/Si(557) [1], the dispersion for Au/Si(553) and Au/Si(775) is also linear for $k_{||} > 0.07\,\text{Å}^{-1}$, a typical signature in 1D. Compared to Au/Si(557) the slope is decreased by a factor of about 2, reflecting the lower electron density of $1 \times 10^7\,\text{cm}^{-1}$. For lower $k_{||}$ the dispersion relations saturate at 200 meV (150 meV) for Au/Si(553) (Au/Si(775)), indicative of quantum well states perpendicular to the steps expected for electronically well separated wires [2].

[1] T. Nagao et al., Phys. Rev. Lett. 97(11), 116802 (2006).

[2] U. Krieg et al., J. Phys.: Condens. Matter 25(1), 14013 (2013)

TT 115.12 Fri 12:45 H 2032

Structural Fluctuations on Si(553)-Au — •Ingo Barke[1], Stefan Polei[1], Paul C. Snijders[2], and Karl-Heinz Meiwes-Broer[1] — [1]University of Rostock, Institute of Physics, 18051 Rostock, Germany — [2]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

The (1x3) reconstruction on Si(553)-Au can be excited to a (1x2) structure by charge injection from the tip of a scanning tunneling microscope [1,2]. Time-resolved measurements enable access to the system's dynamics revealing rapid fluctuations due to a competition between excitation and decay. In this contribution we focus on the time-dependent response to the specific charge injection site. Two distinct locations of high excitation efficiency are identified. This site specific behavior is also found in spatially resolved current-distance curves which are further employed for a quantitative analysis of the current-dependent structural transition of this system. The results are discussed in view of structural and electronic ground state properties of Si(553)-Au.

[1] S. Polei, P.C. Snijders, S.C. Erwin, F.J. Himpsel, K.-H. Meiwes-Broer, and I. Barke, Phys. Rev. Lett. 111, 156801 (2013).

[2] S. Polei, P.C. Snijders, K.-H. Meiwes-Broer, and I. Barke, Phys. Rev. B 89, 205420 (2014).

TT 115.13 Fri 13:00 H 2032

Tb silicide nanowires on Si(001) - a one-dimensional metal? — •Stephan Appelfeller, Martin Franz, Christopher Prohl, Jan Grosse, Zeno Diemer, and Mario Dähne — Inst. f. Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin

Rare earth metals are well known for their formation of metallic bulk silicides with low Schottky-barrier heigths to *n*-type Si. Using appropriate preparation conditions, some rare earth metals, e.g. Tb, are forming silicide nanowires on Si(001) by self-assembly, which have widths of only a few nanometers and lengths of several hundred nanometers. Here, the structural and electronical properties of Tb silicide nanowires are elucidated.

The structural information gained by scanning tunneling microscopy indicates that the Tb silicide nanowires consist of metallic hexagonal $TbSi_2$. Scanning tunneling spectroscopy confirms this finding by showing metallic behavior. Furthermore, angle resolved photoemission data obtained at the UE56/2 PGM1 beamline of BESSY clearly reveal a one-dimensional metallic band structure without dispersion perpendicular to the nanowire main axis. Thus, Tb silicide nanowires are promising for future investigations of unique phenomena of one-dimensional metals, such as the Peierls transition.

This work was supported by the DFG, FOR 1700, project E2. We kindly acknowledge the support of K. Horn and coworkers and of BESSY.

TT 116: Spintronics (incl. Quantum Dynamics) (jointly with MA, HL)

Time: Friday 9:30–12:00 Location: EB 202

Invited Talk TT 116.1 Fri 9:30 EB 202

Antiferromagnetic spintronics — •Tomas Jungwirth — Institute of Physics v.v.i., ASCR, Prague, Czech Republic

Atiferromagnets (AFMs) have for decades played a passive role in conventional spin-valve structures where they provide pinning of the reference ferromagnetic layer. This implies that on one hand, incorporation of some AFM materials in common spintronic structures is well established. On the other hand, limiting their utility to a passive pinning role leaves a broad range of spintronic phenomena and functionalities based on AFMs virtually unexplored. Apart from the insensitivity to magnetic fields and the lack of stray fields, AFMs are common among metals, semiconductors, and insulators and can have orders of magnitude shorter spin-dynamics timescales, to name a few immediate merits of the foreseen concept of AFM spintronics. Several non-relativistic and relativistic spin-transport phenomena have been proposed for AFMs to complement or replace ferromagnets in active parts of spintronic devices. We will focus on the theory of relativistic phenomena and their utility in experimental AFM magneto-resistors, memories, and structures in which AFMs are employed to control ferromagnets electrically.

J. Zelezny et al., Phys. Rev. Lett. 113 (2014) 157201 I. Fina et al., Nature Commun. 5 (2014) 4671 X. Marti et al., Nature Mater. 13 (2014) 367 P. Wadley et al., Nature Commun. 4 (2013) 2322 B.G. Park et al., Nature Mater. 10 (2011) 347

TT 116.2 Fri 10:00 EB 202

Stability of a single spin against readout — •Christoph Hübner[1], Benjamin Baxevanis[1,2], Alexander A. Khajetoorians[3,4], and Daniela Pfannkuche[1] — [1]I. Institute for Theoretical Physics, Hamburg University, Hamburg, Germany — [2]Lorentz Institute, Leiden University, Leiden, The Netherlands — [3]Institute of Applied Physics, Hamburg University, Hamburg, Germany — [4]Institute of Applied Physics, Radboud University Nijmegen, Nijmegen, The Netherlands

A magnetic atom or cluster is extremely sensitive to interactions with a scanning tunneling microscope (STM), that is used to read and write the magnetic state [1]. On the other hand the symmetry of the substrate allows magnetic adatoms to retain their magnetization for minutes, which is extremely long on an atomic time scale [2]. We systematically study this protection against magnetization fluctuations in the presence of a magnetic field and scattering with electrons from the STM and substrate with a non-equilibrium master equation. A combination of spin and substrate symmetry is proposed that produces a stable magnetic orientation even in the presence of a magnetic field [3].

Additionally characteristic features are presented that allow to deduce the spin and substrate symmetry by measurement.

[1] A. A. Khajetoorians et al., Science 339, 55 (2013)
[2] T. Miyamachi et al., Nature 503, 242 (2013)
[3] C. Hübner et al., Phys. Rev. B 90, 155134 (2014)

TT 116.3 Fri 10:15 EB 202

Electric field as a tool for tuning quantum entanglement in supported clusters — •Oleg O. Brovko, Oleg V. Farberovich, and Valeri S. Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Electric field has been recently gaining in reputation as a versatile tool for tuning adsorption, electronic and magnetic properties of nanostructures. In the present contribution we show that using this tool it is also possible to tune quantum entanglement of spins in small clusters on metallic surfaces. Relying on a combination of ab initio and Heisenberg-Dirac-Van Vleck quantum spin Hamiltonian calculations we show by the example of a typical transitional metal dimer (Mn) on Ag(001) surface, that in an inherently unentangled system, electric field can "switch on" the entanglement and change its critical temperature parameter by orders of magnitude. The physical mechanism allowing such rigorous control of entanglement by electric field is shown to be the field- induced change in the internal coupling of the supported nanostructure.

TT 116.4 Fri 10:30 EB 202

Transmission through correlated Cu_nCoCu_n heterostructures — •Liviu Chioncel[1], Cristian Morari[2], Ivan Runger[3], Andrea Drogetti[3], Andreas Oestlin[4], Ulrich Eckern[5], and Andrei Postnikov[6] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D - 86135 Augsburg, Germany — [2]National Institute for Research and Development of Isotopic and Molecular Technologies, 65-103 Donath, RO-400293 Cluj Napoca, Romania — [3]School of Physics and CRANN, Trinity College, Dublin 2, Ireland — [4]Department of Materials Science and Engineering, Applied Materials Physics, KTH Royal Institute of Technology, Stockholm SE - 100 44, Sweden — [5]Theoretical Physics II, Institute of Physics, University of Augsburg, D - 86135 Augsburg, Germany — [6]LCP-A2MC, Institute Jean Barriol, University of Lorraine 1, Bd Arago, F - 57078 Metz, France

We study the effects of local electronic interactions and finite temperatures upon the transmission across the Cu_4CoCu_4 metallic heterostructure in a combined density functional and dynamical mean field theory. We show that the total transmission at the Fermi level is reduced as the electronic correlations are taken into account via a local but dynamic self-energy, whereby such a reduction is more pronounced in the minority spin channel. Consequently, the spin polarization of the transmission increases. Our results also demonstrate that the enhancement in spin contrast is in mainly driven by interaction rather than finite temperature fluctuations.

TT 116.5 Fri 10:45 EB 202

Tricky details of tunnel magnetoresistance — •Christian Franz, Michael Czerner, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University, Giessen, Germany

The basic mechanism responsible for the large TMR in coherent tunnel junctions has already been clarified in the first publications [1,2]. These predictions initiated a broad investigation continuing for more than a decade. Nevertheless, the quantitative understanding of TMR is still incomplete. In particular, the agreement between experiments and calculations remains deficient. The reason for these shortcomings is a complicated interplay of many effects, several of which are not yet fully understood.

We contribute by investigating several effects in great detail using advanced *ab initio* methods [3]. In particular, we discuss the effects of disorder, several interface resonance states and bulk states of different materials. These effects are illustrated by the example of $Fe_{1-x}Co_x$ alloys as ferromagnetic layers [4] which show substitutional disorder for finite concentrations, a complicated concentration dependence of the interface resonance states and variety of bulk states which become available via band filling.

[1] W.H. Butler, X.-G. Zhang, T.C. Schulthess, J.M. MacLaren, Phys. Rev. B 63, 054416 (2001)
[2] J. Mathon, A. Umerski, Phys. Rev. B 63, 220403 (2001).
[3] C. Franz, M. Czerner, C. Heiliger, J. Phys.: Condens. Matter 25, 425301 (2013).
[4] C. Franz, M. Czerner, C. Heiliger, Phys. Rev. B 88, 094421 (2013).

TT 116.6 Fri 11:00 EB 202

Electronic transport in carbon nanotube quantum dots functionalized with magnetic molecules — •Carola Meyer[1,2], Claire Besson[1,2], Michael Schnee[1,2], Henrik Flötotto[3], Robert Frielinghaus[1,2], Lothar Houben[2,4], Paul Kögerler[2,3], and Claus M. Schneider[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technologies, Germany — [3]RWTH Aachen University, Institute for Inorganic Chemistry, 52074 Aachen, Germany — [4]Ernst Ruska-Center for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, 52425 Jülich, Germany

Transport devices built from individual functionalized carbon nanotubes (CNTs) show great potential for instance in spintronics applications. We graft magnetic complexes to CNTs [1]. The route for the CNT functionalization is very general, based on ligand exchange, and can be applied for different molecules, in particular SMMs. We present first quantum transport measurements on individual functionalized CNTs that prove only weak distortion of the electron wave function by the covalent functionalization. The g-factor of the chemically modified CNT quantum dot (QD) is much smaller compared to pristine CNT QDs indicating spin interaction between the QD and the attached molecules. A clear random telegraph signal is recorded depending on the states of the QD. Origin of timescale and energy of the signal are discussed. [1] Meyer, C. et al., Phys. Status Solidi B 249, 2412(2012)

TT 116.7 Fri 11:15 EB 202

Spin transport and its gate-induced modulation in non-degenerate Si at room temperature — •Masashi Shiraishi[1], Tomoyuki Sasaki[2], Yuichiro Ando[1], Makoto Kameno[1], Hayato Koike[2], Toshio Suzuki[3], and Tohru Oikawa[2] — [1]Kyoto Univ., Japan — [2]TDK Corporation, Japan — [3]AIT, Akita Prefectural Industrial Center, Japan

Si spintronics has been collecting tremendous attention, because of its long spin lifetime and achievement of spin transport at room temperature (RT) [1,2]. In the course of our study in Si spintronics, we have revealed that the so-called 3-terminal method [3] cannot completely preclude spurious signals [4], which is now widely recognized [5-7]. Here, we introduce some methods enabling to avoid detection of spurious signals, and report on reliable RT spin transport in non-degenerate n-type Si and gate-induced modulation of spin signals [8]. This is the first experimental demonstration of spin MOSFET at RT, which can pave a way to establish spin-based logic systems.

[1] T. Suzuki, T. Sasaki, M. Shiraishi et al., Appl. Phys. Express 4, 023004 (2011). [2] E. Shikoh, M. Shiraishi et al., Phys. Rev. Lett. 110, 127201 (2013). [3] S. Dash et al., Nature 462, 491 (2009). [4] Y. Aoki, M. Shiraishi et al., Phys. Rev. B86, 081201(R) (2012). [5] O. Txoperena et al., Appl. Phys. Lett. 102, 192406 (2013). [6] T. Uemura et al., Appl. Phys. Lett. 101, 132411 (2012). [7] O. Txoperena, H. Dery et al., Phys. Rev. Lett. 113, 146601 (2014). [8] T. Sasaki, M. Shiraishi et al., Phys. Rev. Applied 2, 034005 (2014).

TT 116.8 Fri 11:30 EB 202

Spin transfer by pure spin current at magnetic interfaces — •Wei Chen[1], Manfred Sigrist[2], Jairo Sinova[3], and Dirk Manske[1] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]ETH-Zurich, Zurich, Switzerland — [3]Johannes Gutenberg University-Mainz, Mainz

We present a microscopic theory for the spin transfer torque, spin pumping, spin mixing conductance, and Onsager relation caused by the pure spin current in the normal metal/ferromagnetic insulator bilayer (such as Pt/YIG) and normal metal/ferromagnetic metal/oxide trilayer (such as $Pt/Co/AlO_x$). The spin Hall effect in the normal metal generates a pure spin current which, upon quantum tunneling into the ferromagnet, causes the magnetization dynamics. The field-like and damping-like component of these spin-transfer quantities are expressed in terms of characteristic energy scales such as the insulating gap and $s-d$ hybridization, which are applicable to a wide range of materials, hence the result can guide the search for materials that have a particular function in spin transport.

TT 116.9 Fri 11:45 EB 202

Spin pumping experiments in Gadolinium Iron Garnet/Pt thin films — Johannes Lotze[1], •Kathrin Ganzhorn[1], Stephan Geprägs[1], Francesco Della Coletta[1], Rudolf Gross[1,2,3], and Sebastian T. B. Goennenwein[1,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Ger-

many — [2]Physik-Department, TU München, Garching, Germany — [3]Nanosystems Initiative Munich, München, Germany

Magnetically compensated rare earth garnets, such as Gadolinium Iron Garnet ($Gd_3Fe_5O_{12}$, GdIG), exhibit a pronounced temperature dependence of the sublattice magnetizations, leading to a magnetization compensation temperature $T_{\mathrm{comp,\,M}}$. The investigation of spin currents in GdIG/Pt heterostructures thus can give important insight into the processes involved in the spin current generation in ferrimagnetic insulator/Pt bilayers. Temperature dependent spin Seebeck effect experiments have recently been performed in GdIG/Pt thin film samples [1], revealing two sign changes of the spin Seebeck voltage, a first one at $T_{\mathrm{comp,\,M}}$ and a second one at a lower temperature. We have performed microwave heating induced spin Seebeck together with spin pumping measurements as a function of temperature in doped GdIG/Pt heterostructures. Our experiments confirm the temperature dependent evolution of the spin Seebeck voltage reported in Ref. [1]. We critically discuss this evolution and compare it to the temperature dependence of the spin pumping voltage observed.

Financial support by DFG via SPP 1538 is gratefully acknowledged.

[1] S. Geprägs *et al.*, arXiv 1405.4971 (2014)

TT 117: Graphene: Intercalation (jointly with O, HL)

Time: Friday 10:30–12:45 Location: MA 041

TT 117.1 Fri 10:30 MA 041

Keeping Argon under a Graphene Lid - Argon intercalation between Graphene and Ni(111) — •Florian Späth, Karin Gotterbarm, Christoph Gleichweit, Max Amende, Udo Bauer, Oliver Höfert, Hans-Peter Steinrück, and Christian Papp — Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

Graphene with its thickness of only one single atomic layer can be considered as the thinnest membrane or gas barrier. We present a spectroscopic investigation of related properties under well-defined ultra-high vacuum conditions in a surface science experiment: We implant argon into a Ni(111) crystal by sputtering prior to the growth of graphene. Subsequently, when growing graphene on Ni(111), argon diffuses out of the bulk and is caught underneath graphene. We investigate the system with high-resolution in-situ X-ray photoelectron spectroscopy. From the growth behavior of these intercalated argon bubbles during graphene preparation and from temperature programmed XP spectra we are able to deduce a model of the intercalation system (G/Ar/Ni) and estimate the pressure for argon under graphene. Furthermore, we find an increased thermal stability of graphene due to a decoupling of graphene from the Ni(111) substrate. This work was supported by SFB 953 "Synthetic Carbon Allotropes"

TT 117.2 Fri 10:45 MA 041

Intercalation of Gadolinium underneath graphene on SiC(0001) — •Stefan Link, Stiven Forti, Alexander Stöhr, and Ulrich Starke — Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

Investigating the properties of graphene in a highly doped state, such that the Fermi level reaches a saddle point of it's electronic bands is an on-going field. Superconductivity could be one potential effect in this regime. Functionalization with highly reactive species such as alkali and/or earth alkali atoms has been pursued for strong doping effects. However, such systems are prone to fast degradation by environmental influences which needs to be circumvented for any kind of application.

Here, we present a method of doping graphene to such levels and simultaneously making the system stable to temperatures higher than 1000°C as well as to air exposure. This was achieved by the intercalation of Gadolinium atoms underneath the so-called buffer layer on SiC(0001), i.e., the carbon rich $(6\sqrt{3}\times6\sqrt{3})$R30° reconstruction of this surface. Significant hybridization effects of the graphene π-bands with the adatom states are observed in the ARPES data. In addition, evidence for strong electron-phonon scattering is visible. Spectroscopic weight appears in the measurements completely interlinking two Dirac cones through the $\overline{\mathrm{M}}$-point, thus indicating the presence of an electronic topological transition (ETT).

TT 117.3 Fri 11:00 MA 041

Nitrogen Intercalation and Nitrogen-based Molecular Doping of Epitaxial Graphene on 6H-SiC(0001) — •Nuala Mai Caffrey, Rickard Armiento, Rositsa Yakimova, and Igor Abrikosov — Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping, Sweden

The thermal decomposition of silicon carbide (SiC) is one of the most promising methods to produce high-quality epitaxial graphene on a wafer scale. Sufficient control has even been achieved to selectively grow monolayer, bilayer and few-layer graphene, rendering it a indispensable technique for the manufacture of graphene-based electronics. A disadvantage of this method is that the first carbon layer is covalently bonded to the surface Si atoms, with only subsequent layers displaying the characteristic electronic features of graphene. Several methods have been proposed to electronically decouple this buffer layer, as well as to reduce the high substrate-induced doping, including intercalation and chemical doping. Understanding such chemical functionalisations is a fundamental first step towards engineering the properties of graphene on SiC. It is clear that the graphene layer, as well as the interface between it and the SiC surface, can be significantly influenced by the growth environment. We consider how common environmental dopants can affect the electronic structure of mono- and bilayer graphene grown on a 6H-SiC(0001) substrate. We show, using first-principles calculations, how nitrogen intercalation and nitrogen-based molecular dopants, such as NO2 and NH3, present a promising route to tailor the properties of this system.

TT 117.4 Fri 11:15 MA 041

Investigation of the electrostatic changes induced by metal islands on graphene/SiC(0001) using field-emission resonance spectroscopy with STM — •Anastasia Sokolova[1], Alexander Stöhr[2], Stiven Forti[2], Ulrich Starke[1,2], and M.Alexander Schneider[1] — [1]Solid State Physics, Friedrich-Alexander-University Erlangen-Nuremberg, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Using the Scanning Tunneling Microscope in field-emission resonance spectroscopy mode (FRS-STM) it is possible to map changes of the electrostatic potential in front of the graphene surface at the nanoscale [1]. We investigated the properties of 10 nm-sized metal islands on top of epitaxial graphene on SiC(0001) as well as islands intercalated underneath the graphene layer.

For cobalt and palladium islands on top of graphene we observe a spatially localized shift of the 1st field-emission resonance to higher energy strictly occurring at the topographical step. This is consistent with larger work functions of the metals with respect to that of graphene. In the case of intercalated cobalt islands FRS-STM shows a rise of the 1st field-emission resonance energy of only 150 meV and a spatially delocalized transition. Considering the properties of graphene flakes on an extended Co(0001) surface [2] this suggests negative charge of the capping graphene layer and a positive charge on the cobalt island.

[1] S. Bose *et al* 2010 *New Journal of Physics* **12** 023028
[2] D. Eom *et al* 2009 *Nano Letters* **9** 2844-2848

TT 117.5 Fri 11:30 MA 041

Oxygen orders differently under graphene: new superstructures on Ir(111) — •Antonio J. Martínez-Galera[1], Felix Huttmann[1], Ulrike Schröder[1], Fabian Craes[1], Carsten Busse[1], Vasile Caciuc[2], Nicolae Atodiresei[2], Stefan Blügel[2], and Thomas Michely[1] — [1]Universität zu Köln, II. Physikalisches Institut, Germany — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

Modifying the properties of graphene (Gr) by intercalation of atoms or molecules at the Gr/substrate interface has been proven to be a straightforward and versatile concept. However, the effect of the Gr layer on the ordering of the intercalated material remains much less studied. We present evidence that indeed the Gr cover has a substantial influence on the resulting superstructures of oxygen chemisorbed on Ir(111). As a function of exposure to molecular oxygen and temperature the oxygen adsorbate superstructures on Ir(111) are identified by scanning tunneling microscopy (STM). They are compared to the

ones formed by intercalation in between graphene and Ir(111). For bare Ir(111) we observe O-(2x2) and O-(2x1) structures, thereby clarifying a long-standing debate on the existence of these structures and the role of defects for their stability. For Gr/O/Ir(111) with increasing exposure O-(2x2), O-(R3xR3)-R30, O-(2x1) and O-(2R3x2R3)-R30 superstructures referred to Ir(111) are observed. The (R3xR3)-R30 and (2R3x2R3)-R30 structures were not yet reported and they exist only under Gr. Based on density functional theory (DFT) we discuss the origin of the new adsorbate superstructures under graphene.

TT 117.6 Fri 11:45 MA 041

Oxidation of sulfuric acid intercalated graphite: the role of sulfuric acid and permanganate ions — •Steffen Seiler and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Wet-chemical exfoliation of graphite via Hummers' method [1,2] is a promising route for large-scale graphene production. This solution-based process is carried out in concentrated sulfuric acid and involves several steps: first, graphite is converted into a sulfuric acid–graphite intercalation compound (GIC), then the GIC is transformed into oxidized graphite, graphene oxide (GO) layers are separated in solution by hydrolysis reactions, and finally the GO layers are reduced to graphene [3].
To obtain atomistic insights into the mechanisms of the chemical reactions in liquid sulfuric acid within the confined space between graphene layers we performed Car-Parrinello molecular dynamics (CP-MD) simulations. By changing the coverage of hydroxy and epoxy groups their stabilizing effect on the attack of sulfuric acid (solvent) and $KMnO_4$ (oxidizing agent) molecules was investigated. Furthermore, different carbon atoms on the partly oxidized graphene sheets were attacked to elucidate the most reactive sites.

[1] W. S. Hummers, *J. Am. Chem. Soc.* **80**, 1339 (1958).
[2] D. C. Marcano et al., *ACS Nano* **4**, 4806 (2010).
[3] A. M. Dimiev and J. M. Tour, *ACS Nano* **8**, 3060 (2014).

TT 117.7 Fri 12:00 MA 041

Approaching ideal graphene: The structure of hydrogen- and germanium-intercalated graphene on 6H-SiC(0001) — •F.C. Bocquet[1,2], J. Sforzini[1,2], T. Denig[3], A. Stöhr[3], T.-L. Lee[4], S. Subach[1,2], U. Starke[3], and F.S. Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, 52425 Jülich, Germany — [3]Max Planck Institute for Solid State Research, Heisenbergstraße, 70569 Stuttgart, Germany — [4]Diamond Light Source Ltd, Didcot, OX11ODE, Oxfordshire, United Kingdom

We investigated Quasi-Free-standing Monolayer Graphene epitaxially grown on 6H-SiC(0001) obtained by decoupling the buffer-layer from the Si-terminated surface by hydrogen intercalation (1) or by intercalating one or two monolayers of germanium (2). All three samples show a clear linear dispersion around the K-point, confirming their Quasi-Free-standing character. We used the X-ray standing wave (XSW) technique, combining dynamical diffraction and X-ray photoelectron spectroscopy, to detect the coherent distribution of the chemically different species (Si, C and Ge) at the interface. Based on the lattice parameter of bulk SiC, we accurately determine the vertical height differences between each chemical species. Comparing the overlaps of van der Waals radii between the graphene layer and the topmost intercalating atoms, we conclude on the degree of decoupling of the graphene layers.

TT 117.8 Fri 12:15 MA 041

Bismuth Intercalated Graphene on Iridium Probed by STM and ARPES — •Jonas Warmuth[1], Matteo Michardi[2], Torben Hänke[1], Marco Bianchi[2], Jens Wiebe[1], Roland Wiesendanger[1], Philip Hofmann[2], and Alexander Khajetoorians[3] — [1]Department of Applied Physics, University of Hamburg, Germany — [2]Department of Physics and Astronomy, University of Aarhus, Denmark — [3]Institute for Materials and Molecules, Radboud University, Nijmegen, Netherlands

We report on the investigation of bismuth intercalated graphene grown on Ir(111) by means of STM and ARPES. The STM measurements reveal a complex periodic structure upon Bi intercalation which we attribute to the formation of a $\sqrt{3}$ Bi surface alloy. We characterize the changes to the band structure using ARPES, including the doping effects and the modification to the Dirac dispersion.

TT 117.9 Fri 12:30 MA 041

Enhancement of many-body effects observed on epitaxial monolayer graphene/Au/SiC(0001) — •Stiven Forti[1], Stefan Link[1], Alexander Stöhr[1], Yuran Niu[2], Alexei Zakharov[2], and Ulrich Starke[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart,Germany — [2]Max-Lab, Lund University, Box 118, Lund, S-22100, Sweden

The interaction of graphene with gold atoms has gained high relevance for a series of reasons, from electrical contacts to plasmonics. Here we present the realization of n-type epitaxial monolayer graphene on SiC(0001) via the intercalation of a layer of Au atoms at the heterointerface between the graphene and the SiC substrate. Such a phase exhibits enhanced many-body effects, as observed by ARPES. The plasmaron band is observed and its dispersion is well discernible from the hole-Dirac cone. The effective dielectric constant extracted from the ARPES data is about five times smaller than what is reported in the literature so far. The effectiveness of the intercalation is corroborated by μLEED measurements, which clearly indicate a suppression of the diffraction spots on the $(6\sqrt{3} \times 6\sqrt{3})$R30° grid, except for spots arising from multiple diffraction. CLPES measurements indicate the presence of a single gold component, namely assigned to gold silicides. The quality of the epitaxial graphene grown on SiC(0001) in Ar atmosphere, together with the aforementioned preparation, makes possible to observe bands of unprecedent sharpness for this system. Dispersive states arising from the 5d orbitals of the interfacial gold are observed as well, as predicted by theory.