Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

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Overview of Invited Talks and Sessions

(Lecture Rooms HSZ 03, HSZ 103, HSZ 201, HSZ 204, HSZ 304; Poster P2)

Invited Talks not included in Focus Sessions and Symposia

TT 2.6	Mon	11:00–11:30	HSZ 103	**The Echo of Superconductivity: Higgs Oscillations of Superconductors in Non-Equilibrium** — •Dirk Manske
TT 14.6	Mon	16:30–17:00	HSZ 201	**Multi-Terminal Josephson Junctions as Topological Matter** — •Julia S. Meyer
TT 12.9	Mon	17:15–17:45	HSZ 03	**U(1) Quantum Spin Liquid Ground State in the Triangular Antiferromagnet $YbMgGaO_4$** — •Yuesheng Li
TT 47.1	Wed	15:00–15:30	HSZ 103	**Interplay between CDW and Superconductivity: Effect of Pressure** — •Matthieu Le Tacon
TT 62.7	Thu	11:15–11:45	HSZ 304	**Optical Control of Complex Quantum Materials** — •Stefan Kaiser
TT 70.1	Thu	15:00–15:30	HSZ 103	**New Developments in the Theory of STM on Unconventional Superconductors** — •Andreas Kreisel

Focus Sessions

"Frustration in Mott Insulators and Mott Criticality"

TT 1.1	Mon	9:30–10:00	HSZ 03	**Herbertsmithite and the Search for the Quantum Spin Liquid** — •Michael Norman
TT 1.2	Mon	10:00–10:30	HSZ 03	**Anisotropic Magnetism and Spin Gap in α-$RuCl_3$** — •Bernd Büchner
TT 1.3	Mon	10:30–11:00	HSZ 03	**The Fate of Spinons in Quantum Critical Mott Systems** — •Vladimir Dobrosavljevic
TT 1.4	Mon	11:15–11:45	HSZ 03	**Breakdown of Hooke's Law of Elasticity at the Mott Critical Endpoint in an Organic Conductor** — •Elena Gati
TT 1.5	Mon	11:45–12:15	HSZ 03	**The Widom Line in Pristine Mott Insulators: Dynamical Properties of Quantum Spin Liquids** — •Andrej Pustogow
TT 1.6	Mon	12:15–12:45	HSZ 03	**Toward Understanding the Complex Magnetism in Kitaev Spin-Liquid Candidates** — •Stephen Winter

"Nematicity, Magnetism and Superconductivity in FeSe and Related Compounds"

TT 21.1	Tue	9:30–10:00	HSZ 03	**BCS-BEC Crossover, Preformed Pairs and Highly Spin-Polarized Superconducting Phase in FeSe** — •Yuji Matsuda
TT 21.2	Tue	10:00–10:30	HSZ 03	**Discovery of Orbital-Selective Cooper Pairing in FeSe** — •J. C. Séamus Davis
TT 21.3	Tue	10:30–11:00	HSZ 03	**Frustrated Magnetism and Electron-Electron Interactions in FeSe** — •Roser Valenti
TT 21.4	Tue	11:15–11:45	HSZ 03	**Orbital-Selective Pairing and Gap Structures of Iron-Based Superconductors** — •Brian Andersen
TT 21.5	Tue	11:45–12:15	HSZ 03	**New Experimental Results Concerning the Nematic State in Fe-based Superconductors** — •Christoph Meingast

"Collective Quantum Dynamics: From Fundamentals to New Phenomena"

TT 46.1	Wed	15:00–15:30	HSZ 03	**Many-Body Localization and Glassiness in Quantum Spin Systems** — •Antonello Scardicchio
TT 46.2	Wed	15:30–16:00	HSZ 03	**Exploring Many-Body Localization in Two Dimensions** — •Christian Gross
TT 46.3	Wed	16:00–16:30	HSZ 03	**Floquet Engineering and Control of Topology in Solid State Systems** — •Takashi Oka
TT 46.4	Wed	16:45–17:15	HSZ 03	**Hydrodynamic Regimes of Electron Transport** — •Andrew Mackenzie
TT 46.5	Wed	17:15–17:45	HSZ 03	**Dynamical Phase Transitions** — •Stefan Kehrein

"Superconductivity in the Vicinity of a Quantum Critical Point"

TT 69.1	Thu	15:00–15:30	HSZ 03	**The Antiferromagnet $YbRh_2Si_2$ - a New Heavy-Fermion Superconductor** — •Frank Steglich
TT 69.2	Thu	15:30–16:00	HSZ 03	**Quantum Criticality in Cuprate and Iron Based Superconductors** — •Antony Carrington
TT 69.3	Thu	16:00–16:30	HSZ 03	**Evolution of the Fermi Surface of the Nematic Superconductors $FeSe_{1-x}S_x$** — •Amalia Coldea
TT 69.4	Thu	16:45–17:15	HSZ 03	**Superconductivity near Structural Instabilities** — •Malte Grosche
TT 69.5	Thu	17:15–17:45	HSZ 03	**An Empirical Approach to the 2 mK Transition in $YbRh_2Si_2$** — •Christoph Geibel

Focus on 2D Materials (Joint Sessions of DS,DY,HL,TT)

Focus Session "Two-Dimensional Materials" (organized by HL)

TT 6.1	Mon	9:30–10:00	POT 81	**Van der Waals Heterostructures: Tunnelling and Interaction with Light** — •Artem Mishchenko
TT 6.6	Mon	11:30–12:00	POT 81	**Excitons in Ultra-Thin Perovskites and van der Waals Crystals** — •Alexey Chernikov
TT 9.1	Mon	14:45–15:15	POT 81	**2D / 3D Heterostructures for Optoelectronis** — •Max Lemme
TT 9.6	Mon	16:45–17:15	POT 81	**Excitons in Colloidal 2D-CdSe Nanocrystals** — •Ulrike Woggon

Focus Session "Ballistic Quantum Transport in Graphene" (organized by TT)

TT 58.1	Thu	9:30–10:00	HSZ 03	**Kondo Screening of a Vacancy Magnetic Moment in Graphene** — •Eva Y. Andrei
TT 58.2	Thu	10:00–10:30	HSZ 03	**Higher-Than-Ballistic Conduction in Viscous Electron Fluids** — •Leonid Levitov
TT 58.3	Thu	10:30–11:00	HSZ 03	**Electron Optics in Ballistic Graphene** — •Ming-Hao Liu
TT 58.4	Thu	11:15–11:45	HSZ 03	**Ballistic Transport in Mesoscopic Graphene Devices** — •Christoph Stampfer
TT 58.5	Thu	11:45–12:15	HSZ 03	**Interaction-Induced Conductance from Zero Modes in a Magnetic Graphene Waveguide** — •Alex Zazunov

Symposium "Optics and Light-Matter Interaction with Excitons in 2D Materials (SYLM)"

See SYLM for the abstracts of the symposium.

SYLM 1.1	Thu	15:00–15:30	HSZ 02	**Light matter interaction in TMDs and their heterostructures** — •Ursula Wurstbauer
SYLM 1.2	Thu	15:30–16:00	HSZ 02	**Quantum optics with deterministically positioned quantum emitters in a two-dimensional semiconductor** — •Brian Gerardot

SYLM 1.3	Thu	16:00–16:30	HSZ 02	**Light-matter coupling with atomic monolayers in microcavities** — •Christian Schneider
SYLM 1.4	Thu	17:00–17:30	HSZ 02	**Properties of Synthetic 2D Materials and Heterostructures** — •Joshua Robinson
SYLM 1.5	Thu	17:30–18:00	HSZ 02	**Exciton spectroscopy in transition metal dichalcogenide monolayers and van der Waals heterostructures** — •Bernhard Urbaszek
SYLM 1.6	Thu	18:00–18:30	HSZ 02	**Strain-induced single-photon emitters in layered semiconductors** — •Rudolf Bratschitsch

Other Joint Symposia with TT participation

Symposium "Novel Functionality and Topology-Driven Phenomena in Ferroics and Correlated Electron Systems (SYCE)"

See SYCE for the abstracts of the symposium.

SYCE 1.1	Mon	15:00–15:30	HSZ 02	**Ferroelectric domain walls: from conductors to insulators and back again** — •Petro Maksymovych
SYCE 1.2	Mon	15:30–16:00	HSZ 02	**Zoology of skyrmions and the role of magnetic anisotropy in the stability of skyrmions** — •Istvan Kezsmarki
SYCE 1.3	Mon	16:00–16:30	HSZ 02	**Magnetic imaging of topological phenomena in ferroic materials** — •Weida Wu
SYCE 1.4	Mon	17:00–17:30	HSZ 02	**Topological skyrmion textures in chiral magnets** — •Markus Garst
SYCE 1.5	Mon	17:30–18:00	HSZ 02	**Learning through ferroelectric domain dynamics in solidstate synapses** — •Manuel Bibes

Symposium "Quantum Optics on the Nanoscale: From Fundamental Physics to Quantum Technologies (SYQO)"

See SYQO for the abstracts of the symposium.

SYQO 1.1	Thu	9:30–10:00	HSZ 02	**Quantum dot based quantum technologies** — •Pascale Senellart
SYQO 1.2	Thu	10:00–10:30	HSZ 02	**Controlled strong coupling of a single quantum dot to a plasmonic nanoresonator at room temperature** — •Bert Hecht
SYQO 1.3	Thu	10:30–11:00	HSZ 02	**High efficiency and directional emission from a nanoscale light source in a planar optical antenna** — •Mario Agio
SYQO 1.4	Thu	11:30–12:00	HSZ 02	**Tailoring quantum states by measurement** — •Jörg Wrachtrup
SYQO 1.5	Thu	12:00–12:30	HSZ 02	**Quantum optics and quantum control at the nanoscale with surface plasmon polaritons** — •Stéphane Guérin

Symposium "Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond (SYES)"

See SYES for the abstracts of the symposium.

SYES 1.1	Fri	10:30–11:00	HSZ 02	**Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations** — •Weitao Yang
SYES 1.2	Fri	11:00–11:30	HSZ 02	**Multi-reference density functional theory** — •Andreas Savin
SYES 1.3	Fri	11:30–12:00	HSZ 02	**Density functionals from machine learning** — •Kieron Burke
SYES 1.4	Fri	12:00–12:30	HSZ 02	**Taming Memory-Dependence in Time-Dependent Density Functional Theory** — •Neepa Maitra
SYES 1.5	Fri	12:30–13:00	HSZ 02	**Quantum Embedding Theories** — •Fred Manby

Sessions

TT 1.1–1.6	Mon	9:30–12:45	HSZ 03	**Focus Session: Frustration in Mott Insulators and Mott Criticality**
TT 2.1–2.11	Mon	9:30–12:45	HSZ 103	**Superconductivity: Properties and Electronic Structure 1**
TT 3.1–3.14	Mon	9:30–13:15	HSZ 201	**Transport: Quantum Dots, Quantum Wires, Point Contacts**
TT 4.1–4.13	Mon	9:30–13:00	HSZ 204	**Transport: Topological Insulators (jointly with DS, MA, HL, O)**
TT 5.1–5.13	Mon	9:30–13:00	HSZ 304	**Correlated Electrons: (General) Theory 1**
TT 6.1–6.9	Mon	9:30–12:45	POT 81	**Focus Session: Two-Dimensional Materials I (joint session DS, HL, TT, organized by HL)**
TT 7.1–7.11	Mon	9:30–13:00	POT 151	**Spintronics I (joint session DS, HL, MA, TT, organized by HL)**
TT 8.1–8.10	Mon	10:30–13:00	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - I (joint session DS, HL, MA, MM, O, TT, organized by O)**
TT 9.1–9.10	Mon	14:45–18:15	POT 81	**Focus Session: Two-Dimensional Materials II (joint session DS, HL, TT, organized by HL)**
TT 10.1–10.7	Mon	14:45–17:00	POT 151	**Spintronics II (joint session DS, HL, MA, TT, organized by HL)**
TT 11.1–11.5	Mon	15:00–18:00	HSZ 02	**SYCE: Novel Functionality and Topology-Driven Phenomena in Ferroics and Correlated Electron Systems (joint symposium DF, DS, KR, MA, MI, TT, organized by DS)**
TT 12.1–12.11	Mon	15:00–18:15	HSZ 03	**Correlated Electrons: Frustrated Magnets - General 1**
TT 13.1–13.12	Mon	15:00–18:15	HSZ 103	**Superconductivity: Fe-based Superconductors - 122**
TT 14.1–14.11	Mon	15:00–18:15	HSZ 201	**Superconductivity: Tunnelling, Josephson Junctions, SQUIDs 1**
TT 15.1–15.12	Mon	15:00–18:15	HSZ 204	**Transport: Graphene and Carbon Nanostructures (jointly with DY, DS, HL, MA, O)**
TT 16.1–16.11	Mon	15:00–18:00	HSZ 304	**Transport: Topological Phases (jointly with DS, MA, HL, O)**
TT 17.1–17.13	Mon	15:00–18:30	HSZ 403	**Magnetic Heuslers, Half-Metals and Oxides (joint session MA, TT, organized by MA)**
TT 18.1–18.12	Mon	15:00–18:15	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - II (joint session DS, HL, MA, MM, O, TT, organized by O)**
TT 19.1–19.70	Mon	15:00–19:00	P2-EG	**Poster Session: Correlated Electrons 1**
TT 20.1–20.21	Mon	15:00–19:00	P2-OG1	**Poster Session: Correlated Electrons 2**
TT 21.1–21.5	Tue	9:30–12:15	HSZ 03	**Focus Session: Nematicity, Magnetism and Superconductivity in FeSe and Related Compounds**
TT 22.1–22.14	Tue	9:30–13:15	HSZ 103	**Transport: Quantum Coherence and Quantum Information Systems - Theory (jointly with MA, HL)**
TT 23.1–23.8	Tue	9:30–11:45	HSZ 201	**Transport: Topological Semimetals 1 (jointly with DS, MA, HL, O)**
TT 24.1–24.13	Tue	9:30–13:00	HSZ 204	**Low-Dimensional Systems: 1D - Theory**
TT 25.1–25.13	Tue	9:30–13:00	HSZ 304	**Correlated Electrons: Frustrated Magnets - Strong Spin-Orbit Coupling 1**
TT 26.1–26.12	Tue	9:30–13:15	POT 51	**Two-Dimensional Materials III (joint session DS, HL, TT, organized by HL)**
TT 27.1–27.7	Tue	9:30–12:45	POT 151	**Focus Session: Topological Insulators on Coupled Quantum Wells (joint session DS, HL, MA, O, TT, organized by HL)**
TT 28.1–28.9	Tue	10:30–13:00	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - III (joint session DS, HL, MA, MM, O, TT, organized by O)**
TT 29.1–29.4	Tue	12:00–13:00	HSZ 201	**Other Low Temperature Topics: Cold Atomic Gases**
TT 30.1–30.8	Tue	14:00–16:00	HSZ 03	**Correlated Electrons: Quantum Impurities, Kondo Physics**
TT 31.1–31.8	Tue	14:00–16:00	HSZ 103	**Correlated Electrons: Other Materials**
TT 32.1–32.5	Tue	14:00–15:15	HSZ 201	**Transport: Nanomechanics and Optomechanics (jointly with CPP, DY, BP, DF)**
TT 33.1–33.8	Tue	14:00–16:00	HSZ 204	**Transport: Majorana Fermions**
TT 34.1–34.7	Tue	14:00–15:45	HSZ 301	**Spintronics, incl. Quantum Dynamics (joint session DS, HL, MA, TT, organized by MA)**

TT 35.1–35.6	Tue	14:00–15:30	HSZ 304	**Low-Dimensional Systems: 2D - Theory**
TT 36.1–36.11	Tue	10:00–13:00	ZEU 147	**Brownian Motion (jointly with DY)**
TT 37.1–37.14	Tue	18:30–20:30	P2-EG	**Graphene Posters (joint session DS, DY, HL, MA, O, TT, organized by O)**
TT 38.1–38.13	Wed	9:30–13:00	HSZ 03	**Transport: Quantum Coherence and Quantum Information Systems - Experiment (jointly with MA, HL)**
TT 39.1–39.14	Wed	9:30–13:15	HSZ 103	**Superconductivity: (General) Theory**
TT 40.1–40.12	Wed	9:30–12:45	HSZ 201	**Transport: Molecular Electronics and Photonics (jointly with CPP, HL, MA, O)**
TT 41.1–41.13	Wed	9:30–13:00	HSZ 204	**Correlated Electrons: Quantum-Critical Phenomena**
TT 42.1–42.13	Wed	9:30–13:00	HSZ 304	**Correlated Electrons: Frustrated Magnets - Strong Spin-Orbit Coupling 2**
TT 43.1–43.13	Wed	9:30–13:15	POT 51	**Two-Dimensional Materials IV (joint session DS, HL, TT, organized by HL)**
TT 44.1–44.5	Wed	10:30–13:00	TRE Phy	**Focus Session: Non-Equilibrium Dynamics in Light-Driven Materials: Theory Meets Experiment (joint session O, TT, organized by O)**
TT 45.1–45.9	Wed	10:30–13:00	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - IV (joint session DS, HL, MA, MM, O, TT, organized by O)**
TT 46.1–46.5	Wed	15:00–17:45	HSZ 03	**Focus Session: Collective Quantum Dynamics: From Fundamentals to New Phenomena**
TT 47.1–47.10	Wed	15:00–18:00	HSZ 103	**Superconductivity: Properties and Electronic Structure 2**
TT 48.1–48.10	Wed	15:00–17:45	HSZ 201	**Superconductivity: Tunnelling, Josephson Junctions, SQUIDs 2**
TT 49.1–49.10	Wed	15:00–17:45	HSZ 204	**Transport: Topological Semimetals 2 (jointly with DS, MA, HL, O)**
TT 50.1–50.11	Wed	15:00–18:00	HSZ 304	**Correlated Electrons: Frustrated Magnets - Low-Dimensional Systems**
TT 51.1–51.10	Wed	15:00–18:00	HSZ 401	**Topological Insulators (joint session DS, HL, MA, O, TT, organized by MA)**
TT 52.1–52.13	Wed	15:00–18:15	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - V (joint session DS, HL, MA, MM, O, TT, organized by O)**
TT 53.1–53.22	Wed	15:00–19:00	P2-OG2	**Poster Session: Superconductivity 1**
TT 54.1–54.9	Wed	15:00–19:00	P2-OG3	**Poster Session: Cryotechnique**
TT 55.1–55.22	Wed	15:00–19:00	P2-OG3	**Poster Session: Superconductivity 2**
TT 56.1–56.18	Wed	15:00–19:00	P2-OG4	**Poster Session: Low-Dimensional Systems**
TT 57.1–57.5	Thu	9:30–12:30	HSZ 02	**SYQO: Quantum Optics on the Nanoscale: From Fundamental Physics to Quantum Technologies (joint symposium HL,DS,O,TT, organized by HL)**
TT 58.1–58.8	Thu	9:30–13:00	HSZ 03	**Focus Session on 2D Materials: Ballistic Quantum Transport in Graphene (jointly with DY, DS, HL, MA, O)**
TT 59.1–59.10	Thu	9:30–12:15	HSZ 103	**Superconductivity: Fe-based Superconductors - FeSe and others**
TT 60.1–60.14	Thu	9:30–13:15	HSZ 201	**Correlated Electrons: f-Electron Systems**
TT 61.1–61.13	Thu	9:30–13:00	HSZ 204	**Correlated Electrons: (General) Theory 2**
TT 62.1–62.12	Thu	9:30–13:00	HSZ 304	**Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 1**
TT 63.1–63.9	Thu	9:30–12:00	HSZ 403	**Spincaloric Transport (joint session MA, TT, organized by MA)**
TT 64.1–64.13	Thu	9:30–13:15	ZEU 160	**Coherent Quantum Dynamics (joint session DY, TT, organized by DY)**
TT 65.1–65.10	Thu	9:30–12:45	POT 251	**Topological Insulators I (joint session DS, HL, MA, O, TT, organized by HL)**
TT 66.1–66.10	Thu	10:30–13:00	WIL A317	**Graphene: Electronic Properties, Structure and Substrate Interaction I (joint session DY, DS, HL, MA, O, TT, organized by O)**
TT 67.1–67.6	Thu	14:45–16:45	POT 251	**Topological Insulators II (joint session DS, HL, MA, O, TT, organized by HL)**

TT 68.1–68.6	Thu	15:00–18:30	HSZ 02	**SYLM: Optics and Light-Matter Interaction with Excitons in 2D Materials (joint symposium DS, DY, HL, TT, organized by HL)**
TT 69.1–69.7	Thu	15:00–18:15	HSZ 03	**Focus Session: Superconductivity in the Vicinity of a Quantum Critical Point**
TT 70.1–70.11	Thu	15:00–18:15	HSZ 103	**Superconductivity: Fe-based Superconductors - Theory**
TT 71.1–71.11	Thu	15:00–18:00	HSZ 201	**Superconductivity: Cryodetectors and Cryotechnique**
TT 72.1–72.13	Thu	15:00–18:30	HSZ 204	**Correlated Electrons: Frustrated Magnets - General 2**
TT 73.1–73.11	Thu	15:00–18:00	HSZ 304	**Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 2**
TT 74.1–74.13	Thu	15:00–18:15	TRE Ma	**Graphene: Electronic Properties, Structure and Substrate Interaction II (joint session DY, DS, HL, MA, O, TT, organized by O)**
TT 75.1–75.32	Thu	15:00–19:00	P2-EG	**Poster Session: Transport 1**
TT 76.1–76.27	Thu	15:00–19:00	P2-OG1	**Poster Session: Transport 2**
TT 77.1–77.9	Thu	16:00–18:30	GER 38	**Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VI (joint session DS, HL, MA, MM, O, TT, organized by O)**
TT 78.1–78.2	Thu	17:00–17:30	CHE 91	**Quantum Optics at the Nanoscale: From Fundamental Physics to Quantum Technologies (joint session HL, DS, O, and TT, organized by DS)**
TT 79.1–79.8	Fri	9:30–11:30	HSZ 03	**Transport: Spintronics, Spincalorics and Magnetotransport (jointly with DS, HL, MA)**
TT 80.1–80.6	Fri	9:30–11:00	HSZ 103	**Low-Dimensional Systems: Oxide Hetero-Interfaces**
TT 81.1–81.4	Fri	9:30–10:30	HSZ 304	**Correlated Electrons: Chiral Magnets**
TT 82.1–82.6	Fri	9:30–11:15	POT 81	**Quantum Information Systems (joint session HL, MA, TT, organized by HL)**
TT 83.1–83.10	Fri	9:30–12:30	POT 251	**Topological Insulators III (joint session DS, HL, MA, O, TT, organized by HL)**
TT 84.1–84.5	Fri	10:30–13:00	HSZ 02	**SYES: Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond (joint symposium DS, HL, MA, MM, O, TT, organized by O)**
TT 85.1–85.10	Fri	10:30–13:00	TRE Ma	**Graphene: Adsorption, Intercalation and Other Aspects (joint session DY, DS, HL, MA, O, TT, organized by O)**
TT 86.1–86.3	Fri	11:15–12:00	HSZ 103	**Low-Dimensional Systems: Charge Order**
TT 87.1–87.4	Fri	11:15–12:15	CHE 89	**Optics and Light-Matter Interaction with Excitons in 2D Materials (joint session HL, DS, O, and TT, organized by DS)**

Annual General Meeting of the Low Temperature Physics Division

Thu 19:00–20:30 HSZ 304

- Report
- Election
- Miscellaneous

TT 1: Focus Session: Frustration in Mott Insulators and Mott Criticality

When electronic correlations drive metals towards Mott insulators, commonly magnetic order occurs. The strong frustration in triangular- and Kagome-lattice Mott insulators, however, may lead to a quantum spin liquid state. In recent years, broad and intense efforts to explore the organic dimer-Mott systems, Herbertsmithite, α-$RuCl_3$ etc. from the experimental and theoretical side led to significant advances in the understanding of frustrated Mott systems, their dynamics, the interplay of charge, spin and orbital degrees of freedom as well as the coupling of the critical electronic system to the lattice degrees of freedom.

Organization: Martin Dressel, Universität Stuttgart; Michael Lang, Universität Frankfurt; Roser Valentí, Universität Frankfurt

Time: Monday 9:30–12:45 Location: HSZ 03

Invited Talk TT 1.1 Mon 9:30 HSZ 03

Herbertsmithite and the Search for the Quantum Spin Liquid — •Michael Norman — Materials Science Division, Argonne National Lab, Argonne, IL 60439 USA

Quantum spin liquids are a novel class of matter where, despite the existence of strong exchange interactions, spins do not order. Typically, they occur in lattices that act to frustrate the appearance of magnetism, the classic example being the kagome lattice composed of corner sharing triangles. There are a variety of minerals whose transition metal ions form such a lattice. Of particular note is herbertsmithite, composed of copper ions forming a kagome lattice. Over the past decade, this material has been extensively studied, yielding a number of intriguing surprises that have in turn motivated a resurgence of interest in the study of the spin 1/2 Heisenberg model on a kagome lattice. In this talk, I will summarize these developments, and then discuss future directions, including the challenge of doping these materials with the hope that this could lead to novel topological or superconducting phases.

Invited Talk TT 1.2 Mon 10:00 HSZ 03

Anisotropic Magnetism and Spin Gap in α-$RuCl_3$ — •Bernd Büchner — IFW Dresden, Helmholtzstraße 20, 01069 Dresden

Quantum spin liquids are a central theme in current condensed matter physics as they host emergent topological order and fractionalized excitations. An important example are interacting Kitaev spins on a honeycomb lattice which are theoretically predicted to exhibit topological and quantum spin liquids. Identifying signatures of Kitaev physics, however, is extremely challenging as real materials, such as the iridates $(Na,Li)_2IrO_3$, inevitably entail an isotropic Heisenberg and additional spin-exchange interactions, thereby stabilizing a magnetically ordered state. Hexagonal Ru trichloride α-$RuCl_3$ has been recently reported to be near the Kitaev spin-liquid phase boundary. The layered honeycomb structure of α-$RuCl_3$ contains layers weakly coupled by van der Waals interaction, i.e. it is a correlated 2d-material offering many possibilities for *materials engineering*. We have characterized the electronic and magnetic properties of α-$RuCl_3$ by a broad spectrum of experimental techniques. From electron spectroscopy basic parameters determining the insulating state of α-$RuCl_3$ are extracted. Moreover, strongly anisotropic magnetic properties as measured from magnetization, specific heat, thermal conductivity, and NMR measurements will be presented and discussed. Both, the behavior of α-$RuCl_3$ in the paramagnetic phase as well as the properties of the ordered state strongly differ from that found in conventional two-dimensional magnets. In particular, we find a very unusual field-temperature phase diagram with evidence for a novel quantum critical point.

Invited Talk TT 1.3 Mon 10:30 HSZ 03

The Fate of Spinons in Quantum Critical Mott Systems — •Vladimir Dobrosavljevic — Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, USA

Recent theoretical and experimental work found evidence of quantum critical scaling behavior around bandwidth-driven Mott transitions in several organic systems of the kappa-family. These experimental results show remarkably universal scaling features, which appear largely identical both in materials displaying long-range antiferromagnetic order on the insulating side, and those showing spin liquid signatures at the lowest temperatures. To provide insight in the role of spin correlations in the critical regime, we blend dynamical mean-field theory (which provided remarkably good description of the high temperature regime), and the RVB-spinon mean-field theory, which describes the spin liquid excitations on the insulating side. Our results indicate that spinon excitations suffer very strong inelastic scattering from dynamical charge fluctuations as soon as the Mott gap closes. We conclude that while spinon excitations dominate the low-temperature insulating regime, they prove largely irrelevant in the entire high-temperature quantum critical regime, in agreement with all available experimental data.

15 min. break.

Invited Talk TT 1.4 Mon 11:15 HSZ 03

Breakdown of Hooke's Law of Elasticity at the Mott Critical Endpoint in an Organic Conductor — •Elena Gati[1], M. Garst[2,3], R.S. Manna[1], U. Tutsch[1], B. Wolf[1], L. Bartosch[4], T. Sasaki[5], H. Schubert[1], J.A. Schlueter[6], and M. Lang[1] — [1]Physikalisches Inst., Goethe Univ., SFB/TR49, Frankfurt, DE — [2]Inst. f. Theo. Physik, Univ. zu Köln, DE — [3]Inst. f. Theo. Physik, TU Dresden, DE — [4]Inst. f. Theo. Physik, Goethe Univ., FFM, DE — [5]IMR, Tohoku Univ., Sendai, Japan — [6]NSF, Arlington, USA

The Mott transition is a prime example of the manifestation of strong electron correlations in solids. Despite its importance for a wide range of materials, however, fundamental properties, such as the universal critical behavior, remain unresolved. An essential, experimentally yet unexplored aspect is the role of electron-lattice coupling on the criticality. In this talk, we will present measurements of the thermal expansion as a function of pressure, P, around the P-induced Mott transition in the organic charge-transfer salt κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl [1]. We observe a breakdown of Hooke's law of elasticity upon approaching the critical endpoint, revealing an intimate, non-pertubative coupling of the critical electronic degrees of freedom to the crystal lattice. Our results are fully consistent with mean-field (MF) criticality, predicted theoretically for electrons in a compressible lattice with finite shear modulus [2]. We argue that every pressure-tunable Mott transition shows the universal properties of an isostructural solid-solid endpoint with MF criticality rather than a liquid-gas endpoint.

[1] Gati *et al.*, Sci. Adv., submitted;
[2] Zacharias *et al.*, PRL **109**, 176401 (12).

Invited Talk TT 1.5 Mon 11:45 HSZ 03

The Widom Line in Pristine Mott Insulators: Dynamical Properties of Quantum Spin Liquids — •Andrej Pustogow[1], Simone Fratini[2], Tsung-Han Lee[3], Vladimir Dobrosavljevic[3], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Institut Néel - CNRS and Université Grenoble Alpes, France — [3]Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, USA

In Mott insulators strong electronic interactions prevent the metallic state. As a paradigm of correlated electron systems, the Mott insulating state is under scrutiny theoretically for more than half a century. Still, the low-temperature behavior evaded experimental exploration because it is typically concealed by an antiferromagnetic phase. In quantum spin liquids, however, no magnetic order is reached, offering the unique possibility to elucidate the pristine Mott state. Here we explore the electrodynamic response of three organic quantum spin liquids with different degrees of effective correlation and frustration. The low-frequency behavior strongly depends on the position in the temperature-pressure phase diagram. In particular in the vicinity of the quantum critical point, metallic fluctuations can be identi-

fied at low temperatures. Combining our optical data with pressure-dependent transport studies and theoretical calculations, we can construct a universal phase diagram of the correlation-controlled Mott insulator.

This work was done in collaboration with M. Bories, E. Zhukova, B. Gorshunov, M. Pinteric, S. Tomic, J. Schlueter, A. Löhle, R. Hübner, T. Hiramatsu, Y. Yoshida, G. Saito and R. Kato.

Invited Talk TT 1.6 Mon 12:15 HSZ 03

Toward Understanding the Complex Magnetism in Kitaev Spin-Liquid Candidates — •Stephen Winter, Kira Riedl, and Roser Valenti — Institut fur Theoretische Physik, Goethe-Universitat Frankfurt

Intensive study of the magnetic response of 5d honeycomb Iridates A_2IrO_3 and 4d α-$RuCl_3$ has been motivated recently by signatures of strongly anisotropic and frustrated interactions reminiscent of the Kitaev spin-liquid. In these materials the complex magnetic interactions arise from a competition between various similar energy scales, including spin-orbit coupling (SOC), Hund's coupling, and crystal-field splitting. Due to this complexity, the interactions in such systems remain hotly debated. In this contribution, we will review the state of the art - the picture that emerges from a combination of ab-initio calculations, microscopic considerations, and analysis of the static magnetic responses. We also discuss the excitation continua observed in a variety of experiments including Raman, neutron, and inelastic x-ray, and conclude that such signatures of fractionalization can persist even far away from the spin-liquid ground state.

TT 2: Superconductivity: Properties and Electronic Structure 1

Time: Monday 9:30–12:45 Location: HSZ 103

TT 2.1 Mon 9:30 HSZ 103

Local probe study of exotic superconductivity via magnetic force microscopy — •Dirk Wulferding[1,2], Hoon Kim[1,3], Ilkyu Yang[1,3], Eric Bauer[4], Joe Thompson[4], Ryan Baumbach[5], Leonardo Civale[4], and Jeehoon Kim[1,3] — [1]CALDES, Institute for Basic Science, Pohang, Korea — [2]IPKM und LENA, TU-BS, Braunschweig, Germany — [3]Dept. of Phys., POSTECH, Pohang, Korea — [4]MPA-CMMS, Los Alamos Natl. Lab., Los Alamos, USA — [5]NHML, Florida State Univ., Tallahassee, USA

Magnetic force microscopy has established itself as a valuable tool to uncover magnetic domain structures on the nanoscale. On the other hand, its magnetically coated tip can serve as an ideal local probe to characterize important properties of superconducting samples [1,2]. We have recently completed designing and constructing a low temperature, ^{3}He magnetic force microscope operating within a three-axis vector magnet [3]. We demonstrate how to employ this system to locally investigate intrinsic properties of the heavy fermion superconductor $CeCoIn_5$, such as the London penetration depth, the pairing symmetry, as well as the pinning force of single Abrikosov vortices.

[1] Kim, et al., Supercond. Sci. Technol. 25, 112001 (2012).
[2] Wulferding, et al., Phys. Rev. B 92, 014517 (2015).
[3] Yang, et al., Rev. Sci. Instrum. 87, 023704 (2016).

TT 2.2 Mon 9:45 HSZ 103

Unexpected rotation of the vortex lattice in the noncentrosymmetric superconductor Ru_7B_3 — •Alistair Cameron[1], Yuliia Tymoshenko[1], Yevhen Onykiienko[1], Aleksandr Sukhanov[1], Geetha Balakrishnan[2], Monica C. Hatnean[2], Don McK. Paul[2], and Dmytro Inosov[1] — [1]Institut für Festkörperphysik, Technische Universität Dresden, Germany — [2]Department of Physics, University of Warwick, Coventry, United Kingdom

Superconductivity in a non-centrosymmetric (NCS) system was first observed in the heavy-fermion compound $CePt_3Si$. This has led to a great deal of interest, as parity is no longer a conserved quantity in a NCS superconductor, leading to a superposition of s-wave and p-wave states. The electronic states around a vortex are strongly influenced by the s+p-wave order parameter, resulting in an anisotropic vortex, which can express itself in the bulk vortex lattice (VL) structure.

We have performed measurements of the VL in the NCS superconductor Ru_7B_3 using small angle neutron scattering. We observe an unusual rotation of the VL with respect to the crystal lattice with changing magnetic field. Normally, a VL selects a single orientation and coordination at any particular magnetic field. However, when changing field below T_c the VL in Ru_7B_3 rotates to a new orientation, dependent not on the absolute field but on the change in field. It is possible that this is due to the Magnus force. However, this is universal to all type-II superconductors, whereas the rotation we observe has not been reported before despite decades of research into vortex matter. We therefore cannot rule out a more exotic origin for our observations.

TT 2.3 Mon 10:00 HSZ 103

Surface state tunneling signatures in two-component superconductor UPt_3 — •Fabian Lambert[1], Alireza Akbari[2,3], Peter Thalmeier[4], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]Asia Pacific Center for Theoretical Physics, Pohang, Gyeongbuk 790-784, Korea — [3]Department of Physics, and Max Planck POSTECH Center for Complex Phase Materials, POSTECH, Pohang 790-784, Korea — [4]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany

Quasiparticle interference (QPI) imaging of Bogoliubov excitations in quasi-two dimensional unconventional superconductors has become a powerful technique for measuring the superconducting gap and its symmetry. Here, we present the extension of this method to three-dimensional superconductors and analyze the expected QPI spectrum for the two-component heavy fermion superconductor UPt_3 whose gap structure is still controversial. Starting from a 3D electronic structure and the three proposed chiral gap models $E_{1g,u}$ or E_{2u}, we perform a slab calculation that determines the 2D continuum Bogoliubov- de Gennes (BdG) surface bands and in addition the in-gap Andreev bound states that lead to surface Weyl arcs connecting the projected gap nodes. Both features are very distinct for the three models, in particular the most prominent E_{2u} candidate is singled out by the existence of two Weyl arcs due to the double monopole nodes. The signature of these distinct surface bound and continuum states provides a fingerprint that may finally determine the true nodal structure of UPt_3.

TT 2.4 Mon 10:15 HSZ 103

Scanning tunneling microscope study of MoN at the superconductor-insulator transition — •Hong Zheng[1], Ina Schneider[2], Christoph Strunk[2], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, Konstanz, Germany — [2]Department of Physics, University of Regensburg, Regensburg, Germany

Superconductor-insulator transition is a phenomenon which has intrigued scientists for several decades. Generally the transition can be induced by magnetic field or decrease of film thickness. Numerous efforts undertaken in a variety of 2D materials reveal remarkable both in the insulating and superconducting state1-4. However, the mechanism behind the transition is still under debate since no theory can explain yet all these experimental findings.

To learn more about the nature of the transition we perform a scanning tunneling microscope study on molybdenum nitride (MoN) thin films close to the superconductor-insulator transition. The fully studied topography shows a disordered structure of MoN thin films whose typical grain size is about 25 nm regardless of the fabrication temperature. In the scanning tunneling spectroscopy of superconducting samples mostly clear gaps and pronounced coherence peaks with slight intensity fluctuations from spot to spot are observed. We will present first result of shot noise measurements of samples whose thickness is very close to the transition point and try to reveal more intrinsic properties besides the topography and spectroscopy information.

TT 2.5 Mon 10:30 HSZ 103

Manipulation of the branching of vortex nucleation in rolled-up superconductor microstructures — E. A. Levchenko[1], R. O. Rezaev[1,2], and •V. M. Fomin[3] — [1]Tomsk Polytechnic University, Tomsk, 634050, Russia — [2]Moscow Engineering Physics Institute, Moscow, 115409, Russia — [3]IFW Dresden, Insitute for Integrative Nanosciences, D-01069 Dresden

An inhomogeneous transport current, which is introduced through multiple electrodes in an open superconductor Nb microtube, is shown to lead to a controllable branching of the vortex nucleation period. The mechanism of this branching is revealed using the time-dependent Ginzburg–Landau equation for the applied magnetic field, which is orthogonal to the axis of the tube. The average number of vortices occurring in the tube per nanosecond can be effectively decreased using the inhomogeneous transport current, which is important for noise and energy dissipation reduction in superconductor applications [1]. The work was supported by the bilateral BMBF-Russia Grant 01DJ13009 and by the COST Action MP1201 "Nanoscale Superconductivity".
[1] R. O. Rezaev, E. A. Levchenko, V. M. Fomin, Supercond. Sci. Technol. **29**, 045014 (2016).

15 min. break.

Invited Talk TT 2.6 Mon 11:00 HSZ 103

The Echo of Superconductivity: Higgs Oscillations of Superconductors in Non-Equilibrium — •Dirk Manske — Max-Planck-Institut für Festkörperforschung

Since the 1:1 analogy of superconductivity with the Higgs mechanism in high-energy physics, the Higgs mode in condensed matter attracted much interest recently [1]. Using Density-Matrix-Theory we predicted in 2008 the existence of Higgs oscillations in superconductors under non-equilibrium conditions. Recently, they have been observed in the optical conductivity of a BCS superconductor using time-resolved pump-probe experiments.

New predictions are made for 2-band superconductors [2] in which 2 Higgs oscillations can not only couple, but also are changing the dispersion of the Leggett mode. This provides a unique coupling between phase and amplitude that can occur only in non-equilibrium.

The nature of Higgs oscillations allows to determine the symmetry of the superconducting order parameter and, thus, marks the way to establish a new 'Higgs spectroscopy' of unconventional superconductors.

[1] D. Manske and M. Dressel, Physik Journal 15, 37 (Jan 2016).
[2] H. Krull et al., Nature Comm. 7, 11921 (2016).

TT 2.7 Mon 11:30 HSZ 103

Observation of an anomalous resistive phase in a strained few-layer $NbSe_2$ crystal — •Andreas Eller, Tobias Scharff, Nicola Paradiso, Sofia Blanter, and Christoph Strunk — Universität Regensburg

We report on an anomalous resistive reentrance in a thin exfoliated crystal of $NbSe_2$. While most of the crystal undergoes a superconducting transition at 5.75 K, a strained region in the middle of it displays a resistive transition at around 4 K. The four-terminal resistance saturates at low temperatures. Similarly to the superconducting phase, the resistive phase can be destroyed by applying a magnetic field. At high bias the superconducting phase and the resistive phase show a dual behavior: while the former is quenched by a critical current, the latter is quenched by a critical voltage. Both the critical voltage for the resistive phase and the superconducting current for the superconducting phase display a similar dependence on temperature and magnetic field.

TT 2.8 Mon 11:45 HSZ 103

Superconducting ferecrystals: turbostratically disordered atomic-scale layered $(PbSe)_{1.14}(NbSe_2)_n$ heterostructures — Corinna Grosse[1], Matti B. Alemayehu[2], Matthias Falmbigl[2], Anna Mogilatenko[3], Olivio Chiatti[1], David C. Johnson[2], and •Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Dept. of Chemistry, University of Oregon, Eugene, Oregon 97403, United States — [3]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, 12489 Berlin, Germany

Hybrid electronic heterostructures of semi- and superconducting layers possess very different properties from their bulk counterparts. Here, we demonstrate superconductivity in ferecrystal films: turbostratically disordered single-, bi- and trilayers of $NbSe_2$ separated by PbSe layers. The turbostratic (orientation) disorder between individual layers does not destroy superconductivity. The artificial sequences of atomic-scale 2D layers are structurally independent of their neighbours in the growth direction. This opens up new opportunities of stacking arbitrary numbers of hybrid superconducting-semiconducting layers in heterostructures which are not available otherwise, because epitaxial strain is avoided. The observation of superconductivity and systematic T_c changes with nanostructure make this synthesis approach of particular interest for realizing hybrid systems in the search of 2D superconductivity and the design of novel electronic hybrid heterostructures.

[1] C. Grosse *et. al*, Scientific Reports **6**, 33457 (2016).

TT 2.9 Mon 12:00 HSZ 103

Superconductivity in $TaSnS_2$ — •Manuel Feig[1,2], Matej Bobnar[2], Walter Schnelle[2], Igor Veremchuk[2], Sergiy Medvediev[2], Andreas Leithe-Jasper[2], and Roman Gumeniuk[1,2] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09596 Freiberg, Germany — [2]MPI für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

The hexagonal $TaSnS_2$ sulphide is reported to be a superconductor with T_c = 2.8 K [1]. However, its superconducting parameters have not been studied up to now. The powder of $TaSnS_2$ was compacted by spark plasma sintering (SPS). The measurements of magnetic susceptibility revealed a superconducting transition at T_c = 2.9 K in agreement with earlier report [1]. The measurements of electrical resistivity and specific heat showed different critical magnetic fields $\mu_0 H_{c2}$ = 22 mT and 200 mT, respectively. This contradiction can indicate an anisotropy of superconducting properties caused by 2H-structure of $TaSnS_2$. The specific heat jump at the transition $\Delta c_p/\gamma T_c = 0.9$ and the energy gap ratio $\Delta(0)/k_B T_c = 1.17$ are well below the values (e.g. 1.43 and 1.76) predicted by BCS theory. This can be again due to an anisotropy of properties or/and by a multigap type of superconductivity. To finally shed light on the superconducting mechanisms in $TaSnS_2$ measurements on oriented crystals are required. High pressure measurements revealed that T_c for $TaSnS_2$ becomes zero for $p > 2.5$ GPa. The Raman measurements indicated a structural phase transition for $TaSnS_2$ above 7 GPa.

[1] J. Dijkastra et al., Phys. Rev. B 40 (1989) 12111.

TT 2.10 Mon 12:15 HSZ 103

Surface reconstructions and Abrikosov lattice in the heavy electron superconductor $TlNi_2Se_2$ — •Stefan Wilfert[1], Martin Schmitt[1], Henrik Schmidt[1], Tobias Mauerer[1], Paolo Sessi[1], Hangdong Wang[2], Qianhui Mao[2], Minghu Fang[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Department of Physics, Zhejiang University, Hangzhou 310027, China

We report on the structural and electronic properties of the heavy electron superconductor $TlNi_2Se_2$. By using a variable-temperature STM various surface $(2 \times n)$ reconstructions were observed which, similar to Fe-based superconductors [1], strongly depend on the temperature during cleavage and the measurement process. Additionally, we performed measurements with a low-temperature STM and found the opening of a superconducting gap. The values for critical temperature and critical magnetic field are in good agreement with earlier transport measurements [2]. In the superconducting state the formation of an Abrikosov lattice was observed without any sign of a zero bias anomaly in the vortex core.

[1] F. Massee *et al.*, Phys. Rev. B **80**, 140507(R) (2009).
[2] H. Wang *et al.*, Phys. Rev. Lett **111**, 207001 (2013).

TT 2.11 Mon 12:30 HSZ 103

Pressure-structure relationships in the 10 K layered carbide halide superconductor $Y_2C_2I_2$ — •Kyunsoo Ahn[1,2], Reinhard K. Kremer[1], Arndt Simon[1], and Alfonso Munoz[3] — [1]MPI for Solid State Research, Stuttgart, Germany — [2]Department of Chemistry, Yonsei University, Wonju 220-710, Korea — [3]Departamento de Física, Instituto de Materiales y Nanotecnología, and MALTA Consolider Team, Universidad de La Laguna, 38200 La Laguna, Tenerife, Spain

In order to investigate to what extend the superconducting and the structural properties of the 10 K layered yttrium carbide halide superconductor $Y_2C_2I_2$ can be modified by external pressure we have studied the pressure dependence of the superconducting critical temperature and the crystal structure of $Y_2C_2I_2$. Up to ∼2.5 GPa. We observe an increase of T_c from 10 K to about 12 K and a structural phase transition from a 1s to a 3s stacking variant. This occurs at ∼2.5 GPa above which T_c rapidly decreases to a value of ∼7.5 K at 7.5 GPa. Ab initio calculations corroborate the structural phase transition to occur at a critical cell volume of ∼270 Å^3 corresponding to a pressure of ∼2.4 GPa, in good agreement with the experimental findings. The pressure dependence of T_c and inter-atomic distances and angles are

discussed with respect to the electronic structure which is characterized by bands of low dispersion and narrow peak-valley features in the electronic density of states at the Fermi level.

TT 3: Transport: Quantum Dots, Quantum Wires, Point Contacts

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

TT 3.1 Mon 9:30 HSZ 201

Unconventional superconductivity in quantum dot systems — •Stephan Weiss and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

For ultra-small quantum dots we study the interplay between spin degrees of freedom and induced superconducting correlations in a nonequilibrium transport setup. Several scenarios of reduced spin symmetry and the consequences for induced even- and odd-frequency order parameters, the Andreev current as well as the shot noise are discussed. Spin symmetry is either reduced by external magnetic fields and/or ferromagnetic leads [1]. Due to the reduced level structure, the single dot case differs from the recently studied double dot system [2].
[1] S. Weiss and J. König, submitted (2016).
[2] B. Sothmann, S. Weiss, M. Governale, J. König, Phys. Rev. B **90**, 220501 (2014).

TT 3.2 Mon 9:45 HSZ 201

Violation of detailed balance for charge-transfer statistics in Coulomb-blockade systems — •Philipp Stegmann and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

We discuss the possibility to generate in Coulomb-blockade systems steady states that violate detailed balance. This includes both voltage biased and non-biased scenarios. The violation of detailed balance yields that the charge-transfer statistics for electrons tunneling into an island experiencing strong Coulomb interaction is different from the statistics for tunneling out. This can be experimentally tested by time-resolved measurement of the island's charge state. We demonstrate this claim for two model systems.
[1] P. Stegmann and J. König, Phys. Status Solidi B (2016), doi:10.1002/pssb.201600507.

TT 3.3 Mon 10:00 HSZ 201

Franck-Condon blockade in driven quantum dots — Patrick Haughian[1], Stefan Walter[2], Andreas Nunnenkamp[3], and •Thomas Schmidt[1] — [1]Physics and Materials Science Research Unit, University of Luxembourg, 1511 Luxembourg, Luxembourg — [2]Institute for Theoretical Physics, University Erlangen-Nurnberg, Staudtstraße 7, 91058 Erlangen, Germany — [3]Cavendish Laboratory, University of Cambridge, Cambridge, CB3 0HE, United Kingdom

Electron-vibron coupling in quantum dots can lead to a strong suppression of the average current in the sequential tunneling regime. This effect is known as Franck-Condon blockade and can be traced back to an overlap integral between vibron states with different electron numbers which becomes exponentially small for large electron-vibron coupling strength. Here, we investigate the effect of a time-dependent drive on this phenomenon, in particular the effect of an oscillatory gate voltage acting on the electronic dot level. We find that the drive can lift the blockade by exciting vibrons. As a consequence, the relative change in average current grows exponentially with the drive strength. We show that this exponential response to a small drive amplitude has important consequences for charge pumping in Franck-Condon blockaded quantum dots.

TT 3.4 Mon 10:15 HSZ 201

Conductance through a helical state in an InSb nanowire — Jakob Kammhuber, Maja Cassidy, Adriaan Vuik, Michal Nowak, •Michael Wimmer, and Leo Kouwenhoven — QuTech and Kavli institute of nanoscience, TU Delft, Netherlands

The interplay of Rashba spin-orbit interaction and Zeeman splitting in nanowires gives rise to a so called "helical state", where carriers with opposite velocity have nearly opposite spins. In particular, this helical state should manifest itself in the quantum point contact (QPC) conductance as a dip in conductance from $2e^2/h$ to $1e^2/h$.

Here, we discuss theoretically how such a helical state can be identified in QPC conductance by rotating the magnetic field. Using this technique, we have found experimental signatures consistent with a helical gap in InSb nanowires, and extracted a value for the spin-orbit coupling strength.

TT 3.5 Mon 10:30 HSZ 201

Noise Properties 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]NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56127 Pisa, Italy

We consider 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 [1]. In this talk we present the current fluctuations. To analyse the rich noise behaviour we calculate the $g^{(2)}$-function and find bunching as well as antibunching of the electrons.
[1] B. Probst, P. Virtanen, and P. Recher, Phys. Rev. B **92**, 045430 (2015).

TT 3.6 Mon 10:45 HSZ 201

Fano stability diagram of a symmetric triple quantum dot — •Michael Niklas, Andreas Trottmann, Andrea Donarini, and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

The Fano factor stability diagram of a C_{3v} symmetric triangular quantum dot is analysed for increasing electron fillings N. At low filling, conventional Poissonian and sub-Poissonian behavior, caused by the interplay of electron-electron interactions and Fermi statistics, is found. At larger filling, $N \geq 2$, super-Poissonian noise and a peculiar bias voltage dependence of the Fano factor are observed at Coulomb and interference blockade. An analysis of the Fano map unravels a nontrivial electron bunching mechanism arising from the presence of degenerate many-body states combined with orbital interference and Coulomb interactions.

TT 3.7 Mon 11:00 HSZ 201

Dark states in spin-resolved transport through triple quantum dots — •Kacper Wrześniewski and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University in Poznań, ul. Umultowska 85, 61-614 Poznań, Poland

We analyze the effect of dark states on spin-dependent transport properties of a triple quantum dot system. The considered quantum dot device is assumed to form a triangular geometry, resembling a simple planar molecule, and is weakly coupled to external ferromagnetic electrodes. The transport characteristics are studied by means of the real-time diagrammatic technique up to the second order of the perturbation theory with respect to the dot-lead coupling.

We examine transport in regimes where both one- and two-electron dark states occur, leading to the current rectification, negative differential conductance and super-Poissonian shot noise. Moreover, we compare the behavior of the tunnel magnetoresistance between different dark state regimes and in Coulomb blockade regime, predicting that the measurement of this quantity may indicate the mechanism of current blockade in similar devices. Finally, we consider the influence of external magnetic field on the formation of dark states and analyze how magnetic field can be used to manipulate coherent population trapping in the system.

15 min. break.

TT 3.8 Mon 11:30 HSZ 201

Levitons in the fractional quantum Hall regime — •L. Vannucci[1], F. Ronetti[1,2], J. Rech[2], D. Ferraro[2], T. Jonckheere[2], T. Martin[2], and M. Sassetti[1] — [1]Università di Genova and CNR-SPIN, Genova, Italy — [2]Aix Marseille Université, Université de Toulon, CNRS, CPT, Marseille, France

Single-electron sources are fundamental building blocks of electron quantum optics, which aims at manipulating electrons one by one in ballistic, coherent conductors. Single-particle excitations above the Fermi sea, devoid of accompanying particle-hole pairs, have been recently spotted through shot noise measurement in a quantum point contact (QPC), following the recipe provided by L. Levitov and collaborators in the '90s (hence the name 'levitons' for such excitations). However, questions can be raised about the robustness of levitons against electron-electron interactions. Here we study levitons in the edge states of the fractional quantum Hall effect (FQHE), where strong Coulombian interactions give rise to exotic quasi-particles with fractional charge and statistic. It is shown that results by Levitov and coworkers are not affected by interactions, since integer levitons still represent minimal excitations states despite the highly non-linear physics occurring at the QPC due to the peculiar collective excitations of the FQHE. We use charge shot noise as well as heat and mixed correlations to shed light on the fascinating properties of Levitov's excitations. In addition, we probe them through Hong-Ou-Mandel (HOM) interferometry. The universal Pauli dip generated by HOM collisions at the QPC further demonstrates the uniqueness of levitons.

TT 3.9 Mon 11:45 HSZ 201

Optimal quantum interference thermoelectric heat engine with edge states — Peter Samuelsson[1], Sara Kheradsoud[1], and •Björn Sothmann[2] — [1]Lund University, 22100 Lund, Sweden — [2]Universität Duisburg-Essen, 47048 Duisburg, Germany

We show theoretically that a thermoelectric heat engine, operating exclusively due to quantum-mechanical interference, can reach optimal linear-response performance. A chiral edge state implementation of a close-to-optimal heat engine is proposed in an electronic Mach-Zehnder interferometer with a mesoscopic capacitor coupled to one arm. We demonstrate that the maximum power and corresponding efficiency can reach 90% and 83%, respectively, of the theoretical maximum. The proposed heat engine can be realized with existing experimental techniques and has a performance robust against moderate dephasing. [1] P. Samuelsson, S. Kheradsoud, B. Sothmann, arXiv:1611.02997 (2016).

TT 3.10 Mon 12:00 HSZ 201

Thermoelectric study of dissipative quantum dot heat engines — Bitan De and •Bhaskaran Muralidharan — Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India

This talk examines the thermoelectric response of a dissipative quantum-dot heat engine [1] based on the Anderson-Holstein model in two relevant operating limits, (i) when the dot phonon modes are out of equilibrium, and (ii) when the dot phonon modes are strongly coupled to a heat bath. In the first case, a detailed analysis of the physics related to the interplay between the quantum-dot level quantization, the on-site Coulomb interaction, and the electron-phonon coupling on the thermoelectric performance reveals that an n-type heat engine performs better than a p-type heat engine. In the second case, with the aid of the dot temperature estimated by incorporating a thermometer bath, it is shown that the dot temperature deviates from the bath temperature as the electron-phonon interactions in the dot become stronger. Consequently, it is demonstrated that the dot temperature controls the direction of phonon heat currents, thereby influencing the thermoelectric performance. Finally, the conditions on the maximum efficiency with varying phonon couplings between the dot and all the other macroscopic bodies are analyzed in order to reveal the nature of the optimum junction.

[1] B. De and B. Muralidharan, Phys. Rev. B, 94, 165416 (2016).

TT 3.11 Mon 12:15 HSZ 201

Dynamic response functions, helical gaps, and fractional charges in quantum wires — •Christopher Pedder[1], Tobias Meng[2], Rakesh P. Tiwari[3], and Thomas L. Schmidt[2] — [1]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [3]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

We show how experimentally accessible dynamic response functions can discriminate between helical gaps due to magnetic field, and helical gaps driven by electron-electron interactions ("umklapp gaps"). The latter are interesting since they feature gapped quasiparticles of fractional charge e/2, and - when coupled to a standard superconductor - an 8π-Josephson effect and topological zero energy states bound to interfaces.

TT 3.12 Mon 12:30 HSZ 201

Spin-dependent scattering in a nanowire — •Alba Pascual[1], Vitaly N. Golovach[1,2,3], Dario Bercioux[2,3], Juan José Sáenz[2,3], and Sebastián Bergeret[1,2] — [1]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU,E-20018 Donostia-San Sebastián, Spain — [2]2Donostia International Physics Center (DIPC), E-20018 Donostia-San Sebastián, Spain — [3]IKERBASQUE, Basque Foundation of Science, E-48011 Bilbao, Spain

We study a quasi-one-dimensional quantum wire in the presence of an impurity and spin-orbit interaction. We solve the problem using a perturbative approach in order to obtain an effective Hamiltonian for the scattering problem. We solve that the scattering problem via the Lippmann-Schwinger equation at the leading order in spin-orbit. We focus on the scattering matrix of a spin-dependent transport setup and elucidate what we believe to be a suitable set of experiments aimed at a scattering matrix tomography.

TT 3.13 Mon 12:45 HSZ 201

Role of incoherent scattering on energy filtering in nanostructured thermoelectric generators — •Aniket Singha and Bhaskaran Muralidharan — Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India

We employ the incoherent non-equilibrium Green's function formalism to investigate in detail the physics of energy filtering and how it leads to an enhancement in power generation across nanostructured thermoelectrics featuring a single planar energy barrier. In particular, we reinforce that the enhancement in the generated power via energy filtering is a characteristic of incoherent scattering and is absent in ballistic devices. By assuming an energy dependent relaxation time, $\tau(E) = kE^r$, we show that there exists a minimum value r_{min} for which the thermoelectric power generation is enhanced and thereby leading to a degradation in power generation for $r < r_{min}$. For bulk generators, we delve into the details of intermode scattering and show that such scattering processes between electrons in higher energy modes and lower energy modes have a finite contribution to the enhancement in the generated power. We also discuss realistic aspects such as finite width of energy barriers and imperfect energy filtering due to partial reflections. In particular, we show that such imperfect filtering and partial transmission of electrons near the top of the barrier affects the enhancement in the generated power drastically in the high efficiency regime of operation.

[1] A. Singha and B. Muralidharan, ArXiv: 1609.07894, (2016)

TT 3.14 Mon 13:00 HSZ 201

Iterative path integral calculation for the interacting resonant level model — Vytautas Abramavicus[1], •Stephan Weiss[2], and Michael Thorwart[3] — [1]Vilnius University, Faculty of Physics, Department of Theoretical Physics, Sauletekio 9, Lithuania — [2]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [3]I. Institut für Theoretische Physik, Universitaät Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany

We calculate the tunneling current through the interacting resonant level model (IRLM) [1] by means of the iterative summation of path integrals (ISPI) scheme. Upon mapping the IRLM to a three dot system [2] with appropriate tunneling and interaction terms, we setup the ISPI scheme for this particluar model. Leads are integrated out exactly and the appearing two interactions of the model are decoupled by two independent Hubbard Stratonovich transformations. The remaining Keldysh path sum is then calculated using the numerically exact ISPI scheme, which relies on the truncation of lead induced correlations after a characteristic memory time τ. We compare our findings to the results of DMRG and fRG calculations.

[1] E. Boulat, H. Saleur, and P. Schmitteckert, Phys. Rev. Lett. **101**, 140601 (2008).

[2] T.J. Suzuki, D.M. Kennes, and V. Meden, Phys. Rev. B **93**, 085306 (2016).

TT 4: Transport: Topological Insulators (jointly with DS, MA, HL, O)

Time: Monday 9:30–13:00 Location: HSZ 204

TT 4.1 Mon 9:30 HSZ 204

Magnetic excitations in the symmetry protected, topological Haldane phase of $SrNi_2V_2O_8$ — Vladimir Gnezdilov[1,2], Vladimir Kurnosov[2], •Peter Lemmens[1], A. K. Bera[3], A. T. M. N. Islam[3], and Bella Lake[3] — [1]TU-BS, Braunschweig — [2]ILTP Kharkov — [3]HZB Berlin

We report results of a single-crystal Raman scattering study of the coupled spin-1 Haldane chain compound $SrNi_2V_2O_8$. In addition to the one-and two-magnon excitations, broad gapless and temperature dependent continua are detected with light polarization parallel to the basal plane. This feature is discussed in terms of spinon-like excitations related to a symmetry protected topological state, of which the Haldane phase in 1D is a preeminent example.

Work supported by RTG-DFG 1952/1, Metrology for Complex Nanosystems and the Laboratory for Emerging Nanometrology, TU Braunschweig.

TT 4.2 Mon 9:45 HSZ 204

Low-temperature magnetotransport in Mn-doped Bi_2Se_3 topological insulators — V. Tkáč[1], V. Komanicky[2], R. Tarasenko[1], M. Vališka[1], V. Holý[1], G. Springholz[3], V. Sechovský[1], and •J. Honolka[4] — [1]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, CZ — [2]Institute of Physics, P. J. Šafárik University, SK — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University, AT — [4]Institute of Physics, Academy of Sciences of the Czech Republic, CZ

Magnetic impurities can break the time-reversal symmetry of 3D topological insulators (TI), thereby opening an energy gap Δ at the Dirac point of a topological surface state with large consequences for transport properties in the thin film limit. In magnetotransport a transition from weak antilocalisation to weak localisation is expected, strongly dependent on contributions from possible coexisting 2D quantum well and bulk states. We present a low-T magnetotransport study ($T = 0.3$ K - 300 K, $B_{max} = 14$ T) of MBE-grown Bi_2Se_3 films of 20 nm - 500 nm thickness with varying Mn concentrations up to 8% and Curie temperatures $T_C = 5-7$ K [1,2]. The results are interpreted following mainly theory by Lu et al. [3] as a competition of quantum corrections to the conductivity σ (phase coherence length $l_\phi \propto T^{-1/2} \sim 50-150$nm for pure Bi_2Se_3) and 2D e-e interaction corrections both in the ferro- and paramagnetic phase.

[1] M. Valiska et al., Appl. Phys. Lett. 108, 262402 (2016).
[2] R. Tarasenko et al., Physica B 481, 262 (2016).
[3] H.-Z. Lu et al., Phys. Rev. Lett. 112, 146601 (2014).

TT 4.3 Mon 10:00 HSZ 204

Proximity-induced superconductivity and quantum interference in topological crystalline insulator SnTe devices — •Robin Klett[1], Joachim Schönle[2], Denis Dyck[1], Karsten Rott[1], Shekhar Chandra[3], Claudia Felser[3], Wolfgang Wernsdorfer[2], and Günter Reiss[1] — [1]CSMD, Bielefeld University, Germany — [2]CNRS, Institut Neél, France — [3]MPI for Chemical Physics of Solids, Germany

Topological states of matter host a variety of new physics that is promising for future technology. Among these phenomena, the emergence of metallic symmetry-protected topological surface states (TSS) are of major interest. The coupling of topological matter to a nearby superconductor is forsaken to host unconventional proximity-induced superconductivity. We demonstrate the fabrication of superconducting Quantum interference devices (SQUIDs) out of SnTe/Nb hybrid structures. Our findings show strong proximity-induced superconductivity in the surface of SnTe. Transport contributions of Majorana Bound States are predicted to enter with a shift in periodicity to DC SQUID experiments. The Analysis of the SQUID response suggest the absence of periodicity shifts, but show additional features expected for TSS carried supercurrents, such as unconventional Fraunhofer shapes.

TT 4.4 Mon 10:15 HSZ 204

Emergence of topological and topological crystalline phases in $TlBiS_2$ and $TlSbS_2$ — •Udo Schwingenschlögl, Qingyun Zhang, and Yingchun Cheng — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

Using first-principles calculations, we investigate the band structure evolution and topological phase transitions in $TlBiS_2$ and $TlSbS_2$ under hydrostatic pressure as well as uniaxial and biaxial strain. The phase transitions are identified by parity analysis and by calculating the surface states. Zero, one, and four Dirac cones are found for the (111) surfaces of both $TlBiS_2$ and $TlSbS_2$ when the pressure grows, which confirms trivial-nontrivial-trivial phase transitions. The Dirac cones at the $\bar{M}$ points are anisotropic with large out-of-plane component. $TlBiS_2$ shows normal, topological, and topological crystalline insulator phases under hydrostatic pressure, thus being the first compound to exhibit a phase transition from a topological to a topological crystalline insulator. [1] Scientific Reports **5**, 8379 (2015)

TT 4.5 Mon 10:30 HSZ 204

Perfect filter for triplet superconductivity on the surface of a 3DTI — •Daniel Breunig[1], Pablo Burset[1], François Crépin[2], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, Wuerzburg University, 97074 Wuerzburg, Germany — [2]Laboratoire de Physique Théorique de la Matière Condensée, UPMC, Sorbonne Universités, 75252 Paris, France

We study a NSN junction on the surface of a 3D topological insulator (TI), where N is a normal region and S is a s-wave proximity-induced superconducting region. Spin-orbit coupling in the TI breaks spin rotational symmetry and induces unconventional triplet superconductivity.

From the anomalous Green function, we identify the singlet and triplet pairing amplitudes and perform a symmetry classification on these quantities. Pauli exclusion principle demands the antisymmetry of the Green function under simultaneous exchange of its space, time and spin variables. The pairing amplitudes can thus be classified as ESE, OSO, ETO or OTE. Here, the first (last) letter specifies the time/frequency (parity) symmetry (Even or Odd) and the second one describes the spin (Singlet or Triplet). A special feature of our system is the emergence of the exotic odd-frequency pairing.

Interestingly, we find that for a bipolar junction, where the chemical potentials in the N leads only differ in their signs, the non-local singlet pairing amplitude is completely suppressed and only triplet pairing occurs. As a result, the non-local conductance across the junction can be dominated by purely spin triplet crossed Andreev reflections, while electron cotunneling is absent.

TT 4.6 Mon 10:45 HSZ 204

Ferromagnetic transition and fluctuation-induced Dzyaloshinskii-Morya interaction at the surface of three-dimensional topological insulators — •Flavio Nogueira[1], Ferhat Katmis[2], and Ilya Eremin[2] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum — [2]Deparment of Physics and Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology

A ferromagnetic insulator (FMI) proximate to the surface of a three-dimensional topological insulator (TI) generate a gap in the spectrum of surface Dirac fermions, provided an out-of-plane exchange exists. We study the ferromagnetic transition in TI-FMI structures and show that fluctuations from Dirac fermions induce a Dzyaloshinskii-Morya (DM) interaction in the effective free energy of the FMI. This DM interaction arises only if the chemical potential is nonzero. Thus, if the proximity effect gaps the Dirac fermions, this means that the Fermi level must be outside the gap in order for a DM term to be induced. We also show that the Curie temperature of the ferromagnetic state at the interface between the TI and FMI is necessarily higher than the bulk Curie temperature of the FMI. This result is corroborated by recent experiments in Bi_2Se_3-EuS bilayer structures. These results imply an interface critical behavior very different from the bulk FMI.

TT 4.7 Mon 11:00 HSZ 204

A time-reversal symmetric topological magnetoelectric effect in 3D topological insulators — •Heinrich-Gregor Zirnstein and Bernd Rosenow — Institut für Theoretische Physik, Universität Leipzig, Germany

One of the hallmarks of time-reversal symmetric (TRS) topological insulators in 3D is the topological magnetoelectric effect (TME). So far, a time-reversal breaking variant of this effect has been discussed, in the sense that the induced electric charge changes sign when the direction

of an externally applied magnetic field is reversed. Theoretically, this effect is described by the so-called axion term. Here, we discuss a time-reversal symmetric TME, where the electric charge depends only on the magnitude of the magnetic field but is independent of its sign. We obtain this non-perturbative result by a combination of analytic and numerical arguments, and suggest a mesoscopic setup to demonstrate it experimentally.

In particular, we show that threading a thin magnetic flux tube of one flux quantum through the material and applying a uniform electric field will induce a half-integer charge $\Delta Q = e/2 \operatorname{sgn} \mathbf{E}_z$ on the surface of the topological insulator. The sign of the induced charge is independent of the direction of the magnetic field.

15 min. break.

TT 4.8 Mon 11:30 HSZ 204

Single-electron injection in the edge states of a 2D topological insulator — •Giacomo Dolcetto and Thomas Schmidt — Physics and Materials Science Research Unit, University of Luxembourg

The realization of single-electron sources in integer quantum Hall systems has paved the way for exploring electronic quantum optics experiments in solid-state devices. Recently, two-dimensional topological insulators have also been considered as an interesting playground for implementing electron quantum optics. Here, two electron waveguides emerge at the edge, one for spin-up and one for spin-down electrons. Scattering between the two channels is strongly suppressed and phase-coherent ballistic transport is predicted. In this talk I will characterize the injection of single Kramers pairs from a mesoscopic capacitor: a periodic voltage drive results in the emission of periodic trains of electron and hole Kramers pairs. Due to spin-momentum locking and to the geometry of the device, the injected state is in general a superposition of many different orthogonal states, thus representing an interesting playground not only to study the transport properties, but also to investigate and to measure the entanglement production.

TT 4.9 Mon 11:45 HSZ 204

Odd-frequency superconductivity at the Helical Edge of a 2D Topological Insulator — •Felix Keidel[1], Pablo Burset[1], François Crépin[2], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, Würzburg University, 97074 Würzburg, Germany — [2]Laboratoire de Physique Théorique de la Matière Condensée, UPMC, Sorbonne Universités, 75252 Paris, France

By virtue of the basic laws of quantum mechanics, the Pauli principle demands the Cooper pairs in superconductors to be odd under exchange of the two constituent electrons. Consequently, even-parity singlets are formed in conventional s-wave superconductivity. Exotic unconventional pairing symmetries emerge once the classification is extended to frequency, additionally to orbital and spin degrees of freedom.

In our work, we study a helical edge of a two-dimensional topological insulator in proximity to an s-wave superconductor and ferromagnetic insulators. While helicity and the magnetic field induce triplet correlations in addition to the inherited singlet pairing, both even- and odd-parity contributions arise since translational invariance and inversion symmetry are broken. In such a hybrid junction, odd-frequency amplitudes thus occur naturally as all combinations of spin and parity symmetry appear. On the basis of a Green's function analysis, we find signatures of these unconventional pairing amplitudes in the local density of states and in the non-local conductance. Strikingly, our method allows to track the emergence of unconventional superconductivity and make a connection to transport and pairing properties of the system.

TT 4.10 Mon 12:00 HSZ 204

Parity anomaly driven topological transitions in magnetic field — •Jan Böttcher, Christian Tutschku, and Ewelina M. Hankiewicz — Institut für Theoretische Physik und Astronomie, Uni Würzburg, 97074 Würzburg, Germany

Recent developments in solid state physics give a prospect to observe the parity anomaly in (2+1)D massive Dirac systems. We show, that the charge neutrality condition for a quantum anomalous Hall (QAH) state in orbital magnetic fields gets modified by an additional term originating from an intrinsic Chern-Simons term in the one loop Lagrangian. This can be utilized to experimentally differentiate the QAH from the quantum Hall (QH) state at charge neutrality [1]. As a result, an experimental signature of the QAH phase in magnetic fields is a long $\sigma_{xy} = e^2/h$ ($\sigma_{xy} = -e^2/h$) plateau in $Cr_x(Bi_{1-y}Sb_y)_{2-x}Te_3$ (HgMnTe quantum wells). Furthermore, we predict a new transition between the quantum spin Hall (QSH) and the QAH state in magnetic fields without magnetic impurities but driven by effective g-factors and particle-hole asymmetry.

[1] J. Böttcher, C. Tutschku, E. M. Hankiewicz, arXiv:1607.07768v1

TT 4.11 Mon 12:15 HSZ 204

Tunable edge states and their robustness towards disorder — •Maik Malki and Götz S. Uhrig — Lehrstuhl für Theoretische Physik 1, TU Dortmund, Germany

The interest in the properties of edge states in Chern insulators and in $\mathbb{Z}_2$ topological insulator has increased rapidly in recent years. We present calculations on how to influence the transport properties of chiral and helical edge states by modifications of the edges in the Haldane and in the Kane-Mele model. The Fermi velocity of the chiral edge states becomes direction-dependent as does the spin-dependent Fermi velocity of the helical edge states. Moreover, it is possible to tune the Fermi velocity by orders of magnitude. Additionally, we explicitly investigate the robustness of edge states against local disorder. The edge states can be reconstructed in the Brillouin zone in presence of disorder. The influence of the width and of the length of the system is studied as well as the dependence on the strength of the disorder.

TT 4.12 Mon 12:30 HSZ 204

Instability of interaction-driven topological insulators against disorder — Jing Wang[1,2], Carmine Ortix[1,3], Jeroen van den Brink[1], and •Dmitri Efremov[1] — [1]IFW Dresden, Germany — [2]University of Science and Technology of China, Hefei, China — [3]Utrecht University, Netherlands

We analyze the effect of disorder on the weak-coupling instabilities of quadratic band crossing point (QBCP) in two-dimensional Fermi systems, which, in the clean limit, display interaction-driven topological insulating phases. In the frame of the weak-coupling renormalization group procedure, which treats fermionic interactions and disorder on the same footing, we test all possible instabilities and identify the corresponding ordered phases in the presence of disorder for both single-valley and two-valley QBCP systems. We find that disorder generally has a strong influence on the stability of the interaction-driven topological insulating phases – it strongly suppresses the critical temperature at which the topologically non-trivial order sets in – and can even trigger a phase transition to different, topologically trivial, ordered phases.

TT 4.13 Mon 12:45 HSZ 204

Effect of disordered geometry on transport properties of three dimensional topological insulator nanowires — •Emmanouil Xypakis[1], Jun Won Rhim[1], Roni Ilan[2], and Jens H. Bardarson[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Department of Physics, University of California, Berkeley, California

Three dimensional topological insulator nanowires are materials which, while insulating in the bulk, have a metallic boundary described by a two dimensional Dirac Hamiltonian with antiperiodic boundary conditions. Transport properties of this system have been extensively studied in the limit where the surface manifold is conformally at (e.g., a cylinder) in the presence of a random disordered scalar potential. In this talk I will discuss how this picture is altered when a more realistic surface manifold is chosen, such as a cylinder with a randomly fluctuating radius.

TT 5: Correlated Electrons: (General) Theory 1

Time: Monday 9:30–13:00 Location: HSZ 304

TT 5.1 Mon 9:30 HSZ 304

Parquet decomposition calculations of the electronic self-energy — Olle Gunnarsson[1], Thomas Schäfer[2], James LeBlanc[3], Jaime Merino[4], Giorgio Sangiovanni[5], Georg Rohringer[6], and •Alessandro Toschi[2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart (Germany) — [2]IFP, Technische Universität Wien (Austria) — [3]Memorial University of Newfoundland, St. John's (Canada) — [4]Universidad Autónoma de Madrid (Spain) — [5]University of Würzburg (Germany) — [6]Russian Quantum Center, Moskow (Russia)

The parquet decomposition of the self-energy into classes of diagrams, those associated with specific scattering processes, can be exploited for different scopes. In our work[1], the parquet decomposition is used to unravel the underlying physics of non-perturbative numerical calculations. By applying DMFT and its cluster extensions to the Hubbard model, our calculations show that the self-energies in the underdoped regime are dominated by spin-scattering processes, consistent with the conclusions of the *fluctuation diagnostics* approach[2]. We find, however, that even for moderate couplings, well before the Mott transition, singularities appear in different terms of the decomposition, with the notable exception of the predominant spin-channel. We clarify how these singularities, which partly limit the utility of parquet-based algorithms, are *never* found in the fluctuation diagnostics procedure.
[1] O. Gunnarsson *et al.*, Phys. Rev. B **93**, 245102 (2016)
[2] O. Gunnarsson *et al.*, Phys. Rev. Lett. **114**, 236402 (2015)

TT 5.2 Mon 9:45 HSZ 304

Impact of nonlocal correlations over different energy scales: A dynamical vertex approximation study — •Georg Rohringer[1] and Alessandro Toschi[2] — [1]Russian Quantum Center, Moscow (Russia) — [2]Technische Universität Wien (Austria)

We investigate [1] how nonlocal correlations affect, selectively, the physics of correlated electrons over different energy scales, from the Fermi level to the band edges. This goal is achieved by the dynamical vertex approximation (DΓA), studying several spectral and thermodynamic properties of the unfrustrated Hubbard model in $2d$ and $3d$. Specifically, we focus first on the low-energy regime by computing the electronic scattering rate and the quasiparticle mass renormalization for decreasing temperatures at a fixed interaction strength. This way, we obtain a precise characterization of the several steps through which the Fermi-liquid physics is progressively destroyed by nonlocal correlations. Our study is then extended to a broader energy range, by analyzing the temperature behavior of the kinetic and potential energy, as well as of the corresponding energy distribution functions. Our findings allow us to identify a smooth but definite evolution of the nature of nonlocal correlations by increasing interaction. Finally, a critical analysis of our numerical results of the potential energy at the largest interaction allows us to identify possible procedures to improve state-of-the-art algorithms beyond DMFT.
[1] G. Rohringer and A. Toschi, Phys. Rev. B **94**, 125144 (2016).

TT 5.3 Mon 10:00 HSZ 304

Breakdown of the many-body perturbation theory: Vertex divergences in the Anderson Impurity Model — •Patrick Chalupa, Patrik Gunacker, Thomas Schäfer, Karsten Held, and Alessandro Toschi — Technische Universität Wien, Karlsplatz 13, 1040 Wien

The recently discovered [1,2] occurrence of multiple divergences in the irreducible vertex functions of strongly correlated electron models, poses serious problems to the state-of-the-art many-body theory. Dynamical mean-field theory calculations for the Hubbard model have shown several lines of divergences, surrounding the Mott-Hubbard metal-insulator transition, a clear hint of a highly non-perturbative origin. At high temperatures/large U, where the Hubbard model approaches the atomic limit, the divergences could be ascribed to a unique underlying energy scale ν^*. This simple picture is however not applicable in the most interesting parameter regime of low temperatures and intermediate U.

For this reason we analysed a simpler model where a similar physics could be realized: the Anderson impurity model. This provides a more feasible way to treat quasiparticle physics in the parameter regime of interest. Our CT-HYB calculations, performed with w2dynamics [3] at the two particle level, extending to even lower temperatures than before, provide novel insight into this topic.
[1] T.Schäfer, *et al.*, 1606.03393, to be published in Phys. Rev. B
[2] T.Schäfer, *et al.*, Phys. Rev. Lett. **110**, 246405 (2013)
[3] N.Parragh, *et al.*, Phys. Rev. B **86**, 155158 (2012)

TT 5.4 Mon 10:15 HSZ 304

Ab initio dynamical vertex approximation — Anna Galler, Patrik Thunström, Patrik Gunacker, •Jan M. Tomczak, and Karsten Held — Institute of Solid State Physics, TU Wien, A-1040 Vienna, Austria

Diagrammatic extensions of dynamical mean field theory (DMFT) such as the dynamical vertex approximation (DΓA) allow us to include non-local correlations beyond DMFT on all length scales and proved their worth for model calculations. Here, we develop and implement an Ab-initio-DΓA approach for electronic structure calculations of materials. Starting point is the two-particle irreducible vertex in the two particle-hole channels which is approximated by the bare non-local Coulomb interaction and all local vertex corrections. From this we calculate the full non-local vertex and the non-local self-energy through the Bethe-Salpeter equation. The Ab-initio-DΓA approach naturally generates all local DMFT correlations and all non-local GW contributions, but also further non-local correlations beyond: mixed terms of the former two and non-local spin fluctuations. We apply this new methodology to the prototypical correlated metal $SrVO_3$.

TT 5.5 Mon 10:30 HSZ 304

Spin-orbit coupling and Hund's physics: The role of effective spin-orbital degeneracy — •Robert Triebl and Markus Aichhorn — Institute of Theoretical and Computational Physics, NAWI Graz, Graz Univerity of Technology, Petersgasse 16, 8010 Graz, Austria

We analyze the mutual influence of spin-orbit coupling and orbital degeneracy on strongly-correlated systems using Dynamical Mean Field Theory (DMFT) on a Bethe lattice. It is known that Hund's coupling leads to qualitatively different behavior, depending on whether the system is at half-filling or not. Here, we show that the notion of half-filling has to be re-considered in the case of strong spin-orbit coupling (SOC). In particular, SOC breaks particle-hole symmetry and lifts orbital degeneracy, because it splits the semicircular density of states into an effective two-band ($j = 3/2$) and an effective one-band ($j = 1/2$) part. Hence, it reduces the number of active orbitals and changes the effective spin-orbital degeneracy. We are analyzing the development of this degeneracy and its influence on the correlation strength as function of spin-orbit and Hund's coupling. Furthermore, the tendencies observed on the Bethe lattice are compared to LDA+DMFT calculations of Sr_2RuO_4 with different spin-orbit couplings.

TT 5.6 Mon 10:45 HSZ 304

Benchmarking MPS-based Time Evolution schemes for low-dimensional interacting quantum systems — •Sebastian Paeckel[1], Thomas Köhler[1], Alexander Tiegel[1], Stephan Kramer[2,1], and Salvatore Manmana[1] — [1]Institut für Theoretische Physik, U. Göttingen — [2]Fraunhofer ITWM, Kaiserslautern

We compare different approaches to compute out-of-equilibrium dynamics with matrix product state (MPS) methods. Traditionally, either a Suzuki-Trotter-decomposition of the time evolution operator, or a projection onto Krylov-space is used. Here, we take into account recent developments which are based on directly applying local matrix product operators (MPO) in a low-order-expansion to the MPS [1], or which involve a global update scheme projecting the variationally time-evolved MPS into its tangent space [2]. The obtained benchmarks are then compared with respect to their numerical stability and efficiency for spin Hamiltonians on chains and ladder geometries.

We gratefully acknowledge financial support by DFG FOR 1807 (project P7) and CRC 1073 (project B03).
[1] M. Zaletel et al., Phys. Rev. B 91, 165112 (2015)
[2] J. Haegeman et al., Phys. Rev. Lett. 107, 070601 (2011)

15 min. break.

TT 5.7 Mon 11:15 HSZ 304

Generic Construction of Efficient Matrix Product Operators — •Claudius Hubig[1], Ian McCulloch[2], and Ulrich Schollwöck[1] — [1]Department of Physics and Arnold Sommerfeld Center for Theoretical Physics,Ludwig-Maximilians-Universität München, Germany — [2]Centre for Engineered Quantum Systems, School of Physical Sciences, The University of Queensland, Brisbane, Australia

Matrix Product Operators (MPOs) are at the heart of the second-generation Density Matrix Renormalisation Group (DMRG) algorithm formulated in Matrix Product State language. We give an introduction to arithmetic with general MPOs and compression of general MPOs. We show that it is possible to generate optimal representations of a wide class of Hamiltonians using a very generic construction method, including powers of short-range one-dimensional Hamiltonians, Hamiltonians for two-dimensional systems and as a proof of principle, the long-range four-body Hamiltonian from quantum chemistry. The construction method consists of the definition of single-site operators, implementation of generic MPO arithmetic for addition and multiplication and the use of three compression methods (Rescaled SVD, Deparallelisation and Delinearisation) to achieve the most efficient MPO representation.

TT 5.8 Mon 11:30 HSZ 304

Fork Tensor Product States - Efficient Three Orbital Real Time DMFT Solver — •Daniel Bauernfeind, Manuel Zingl, Robert Triebl, Markus Aichhorn, and Hans Gerd Evertz — Institute of Theoretical and Computational Physics, Graz, Austria

We present a new tensor network especially suited for multi-orbital Anderson impurity models and, hence, also as an impurity solver for multi-orbital Dynamical Mean-Field Theory (DMFT). The solver works directly on the real-frequency axis, which yields very high spectral resolution at all frequencies. Within this approach one is not restricted by the number of bath sites, and can therefore achieve an accurate representation of the bath. Furthermore, this method can treat full-rotational invariant interactions with reasonable numerical effort. We show the efficiency and accuracy of the method by a benchmark for the testbed material $SrVO_3$. There we observe a multiplet structure in the high-energy Hubbard bands which is almost impossible to resolve by other mulit-orbital methods. We also show that the resulting structure of the Hubbard bands can very well be explained by broadened atomic spectra with rescaled interaction parameters. This impurity solver offers a new route to the calculation of precise real-frequency spectral functions of correlated materials.

TT 5.9 Mon 11:45 HSZ 304

Modeling correlated systems: from atoms to materials — •Qian Zhang and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

The study of strongly correlated materials requires careful treatment of electron-electron interactions. Our starting point is density functional calculations for individual atoms and ions to obtain realistic basis functions. In particular, we focus on the open-shell orbitals, which have the strongest correlation effects. While atomic orbitals are mutually orthogonal within a single atom, they are in general not orthogonal for atoms on different lattice sites. We will discuss multi-center integral techniques for evaluating orbital overlaps, which are essential for performing orbital orthogonalization. This allows us to study atomic orbitals in various crystal structures. To orthogonalize the basis orbitals, we apply the Löwdin symmetric orthogonalization scheme which leads to the minimum orbital modification. For the resulting orbitals, we study the deformation due to orthogonalization, and investigate how the Coulomb matrix elements are changed compared with the atomic ones.

TT 5.10 Mon 12:00 HSZ 304

Band structure induced electronic correlations in nickel and iron: van-Hove singularities vs. Earth's core conditions — •Andreas Hausoel[1], Michael Karolak[1], Ersoy Sasioglu[2], Alexander Lichtenstein[3], Karsten Held[4], Andrey Katanin[5], Alessandro Toschi[4], and Giorgio Sangiovanni[1] — [1]University of Wuerzburg — [2]Research Center Jülich — [3]University of Hamburg — [4]TU Vienna — [5]Institute of Metal Physics Ekaterinburg

Some Bravais lattices have a particular geometry and can slow down the motion of Bloch electrons: a 'pre-localisation' due to band structure properties. Another known source of electronic localisation in solids is the Coulomb repulsion in partially-filled d- or f-orbitals, which leads to the formation of local magnetic moments. The combination of these two effects has been viewed so far as mainly an academic issue. Here we show with ab-initio calculations of unprecedented accuracy and model studies, that their synergy represents instead the underlying physical mechanism in two of the most important ferromagnets: nickel and iron. Furthermore in nickel, the van-Hove singularity is essential for ferromagnetism to appear. nickel's electron-electron scattering rate is linear in temperature, in violation of the conventional Landau theory of metals. This is true even at Earth's-core conditions, at which iron is instead a good Fermi-liquid. The importance of nickel in models of geomagnetism may therefore be reconsidered.

TT 5.11 Mon 12:15 HSZ 304

Non-local screening effects in strongly correlated materials — •Evgeny Stepanov — Radboud University, Institute for Molecules and Materials, 6525AJ Nijmegen, The Netherlands

Dynamical mean-field theory (DMFT) is one of the most popular approaches to strongly correlated systems. It provides an approximate solution of the Hubbard model by mapping it to a local impurity problem. Later, an extended dynamical mean-field theory (EDMFT) was introduced to include collective degrees of freedom into DMFT. Unfortunately, these collective excitations have a strongly non-local nature, so EDMFT is insufficient and it was necessary to develop some extensions to treat non-local correlations. To go beyond EDMFT, one needs to determine the corrections to the electronic self-energy and polarization operator that describe excitations that were not taken into account at the impurity level. Therefore, the great care should be taken to avoid double counting of correlation effects when merging EDMFT with the extension part.

Here we introduce the Dual Boson (DB) approach and show, that existing up to now approaches, such as EDMFT+GW, can be easily derived from the exact dual transformations and should be corrected in order to obtain better physical description of strongly correlated systems. The DB theory is free from double counting problems by construction, therefore, for the same computational complexity as the standard EDMFT+GW approach, the Dual Boson formalism significantly improves physical results and solves the double-counting problem.

TT 5.12 Mon 12:30 HSZ 304

Charge self-consistent LDA+DMFT scheme with energy-dependent orbitals — •Andreas Östlin[1], Levente Vitos[2,3,4], and Liviu Chioncel[5,1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Department of Materials Science and Engineering, Applied Materials Physics, KTH Royal Institute of Technology, SE-10044 Stockholm, Sweden — [3]Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75120 Uppsala, Sweden — [4]Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, P.O. Box 49, H-1525 Budapest, Hungary — [5]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

We propose a new charge self-consistent scheme for the combined density functional and dynamical mean field theory (LDA+DMFT), suitable for energy-dependent orbitals. In the present implementation the many-body effects are incorporated into the Kohn-Sham iterative scheme without the need for the numerically ill-posed analytic continuation of the Green's function and the self-energy. This is achieved by formulating the Kohn-Sham problem directly on the Matsubara axis. We show results from an implementation in the exact muffin-tin orbitals (EMTO) method.

TT 5.13 Mon 12:45 HSZ 304

Efficient implementation of DFT+DMFT for spin-orbit coupled systems — •Gernot J. Kraberger and Markus Aichhorn — Institute of Theoretical and Computational Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

In systems containing heavy atoms with open d-shells, both electronic correlations and spin-orbit coupling (SOC) play an important role. Therefore, both have to be included in a theoretical description of such materials. A very successful way to account for the electron-electron interaction in crystals is the DFT+DMFT. In this contribution, we explain a strategy to tackle all the obstacles one faces when including SOC in this well-established framework.

Typically, SOC leads to significant complex-valued orbital hybridisations that are absent otherwise. As a consequence one has to deal

with matrix valued Green's functions, which causes difficulties for the Monte-Carlo impurity solvers, mainly by a pronounced fermionic sign problem. We show that a carefully chosen basis rotation can drastically improve this issue. But still, the numerical effort increases significantly when accounting for SOC, as the number of internal symmetries is reduced. We present our approach to reduce the degrees of freedom to make prohibitively costly calculations feasible. All these points are illustrated with a layered oxide heterostructure as example system.

TT 6: Focus Session: Two-Dimensional Materials I (joint session DS, HL, TT, organized by HL)

Time: Monday 9:30–12:45 Location: POT 81

Invited Talk TT 6.1 Mon 9:30 POT 81

Van der Waals heterostructures: tunnelling and interaction with light — •Artem Mishchenko — School of Physics and Astronomy, The University of Manchester, Manchester, UK

When graphene or other conducting 2D crystals are separated by an atomically thin insulating 2D crystal (e.g. hexagonal boron nitride), quantum mechanical tunnelling leads to the appreciable interlayer current between the two 2D conductors due to the overlap of their wave functions. These tunnel devices reveal exciting physics and great potential for applications: resonant tunnelling, negative differential conductance, light emission and detection, to name a few. Here, I will update on a current status and perspectives of tunnelling devices and quantum wells based on 2D materials assembled into van der Waals heterostructures. Particularly, I will present the results on tunnelling in mono- and bilayer graphene, tunnelling in 2D crystal-based quantum wells, and tunnelling in superconducting 2D materials. I will overview such effects as momentum and chirality conservation, phonon- and impurity-assisted tunnelling. Furthermore, interaction with light (i.e. photovoltaics, solar cells, light emission, lasing and plasmonics) within these heterostructures will be discussed. Finally, possible practical applications will be outlined.

TT 6.2 Mon 10:00 POT 81

Quantum emission from low dimensional materials — •Nathan Chejanovsky[1,2], Youngwook Kim[2], Andrea Zappe[1], Rainer Stöhr[1], Felipe Favaro de Oliveira[1], Durga Dasari[1,2], Amit Finkler[1], Jurgen H. Smet[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, 70569 Stuttgart, Germany

Quantum emitters (QEs) in semi-conductors are at the forefront of optical research. 3D solid state systems [1] and quantum dots [2] are known sources of QEs. Nevertheless, quantum dots have constraints on temperature operation, broad linewidths and emission intermittency rendering these systems problematic. 3D systems suffer from light scattering and are difficult to process into tailored nano-structures.

Low dimensional wide band-gap materials (e.g. Van der Waals crystals) open possibilities for circumventing these obstacles, accessing intra-band gap states using sub-band gap excitation. Fulfilling this criteria, hexagonal boron nitride (h-BN), hosts room temperature QEs. [3] I summarize developments in this field and present results from our recent publication: [3] connecting structural features and QE location, generation of QEs using chemical etching/ion irradiation and analyzing their spectral features and photodynamics.

[1] Jelezko, F. et al. phys. stat. sol. (a) 2006, 203(13), 3207-3225
[2] Lodahl, P. et al. Reviews of Modern Physics 2015, 87 (2), 347-400
[3] Chejanovsky, N. et al. Nano letters 2016, 16, 7037-7045

TT 6.3 Mon 10:15 POT 81

Layered semiconductors coupled to an optical microcavity — •Michael Förg[1], Hisato Yamaguchi[2], David Hunger[3,4], and Alexander Högele[1] — [1]Fakultät für Physik and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Germany — [2]Materials Physics and Applications Division, Los Alamos National Laboratory, USA — [3]Ludwig-Maximilians-Universität München, Schellingstr. 4, München, Germany — [4]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, Garching, Germany

Two-dimensional atomic crystals of transition metal dichalcogenides exhibit remarkable optoelectronic properties in the limit of direct band-gap monolayers [1]. Bilayer heterostructures, on the other hand, feature long-lived indirect excitons potentially viable for studies of condensation phenomena [2]. In the scope of this work we investigate excitons in CVD grown layered semiconductors coupled to an optical microcavity. In our experiments we use a tunable open-access cavity with one curved fiber-based mirror and one planar mirror which supports laterally extended semiconductor flakes. This configuration allows us to combine controlled inter-mirror spacing with lateral scanning capabilities. While the former parameter is used to explore the light-matter coupling as a function of the cavity length, the latter enables two-dimensional cavity imaging of extended monolayer flakes to probe variations in the local crystal quality and the dielectric environment.

[1] Xu et al., Nat. Phys. 10, 343 (2014)
[2] Rivera et al., Nat. commun. 6 (2015)

TT 6.4 Mon 10:30 POT 81

Understanding single-photon emission from defects in hexagonal boron nitride — •Sten Haastrup and Kristian S. Thygesen — Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark

Point defects in sheets of hexagonal boron nitride have recently been studied as potential single-photon emitters: Experimental studies have shown that the emission from point defect color centers has extremely narrow bandwidth and mainly takes place in the zero phonon line. From an engineering perspective, a high-quality source of single photons would be extremely useful for many applications including quantum computing and quantum communications. Currently, it is not clear which defect systems in boron nitride have the right properties for use as single-photon emitters; different experimental studies have observed emission at very different energies, indicating that multiple different defect states can produce single photons. This is the starting point for our investigation into which properties of defects are important for single-photon emission, and which properties of boron nitride make it suitable as host. We have used density functional theory to explore the potential energy surfaces of the ground- and lowest excited states around different point defects in hBN. Our calculations shed light on the observed narrow band nature of the emission lines and indicate potential routes for tuning emission energy, line width and lifetime.

TT 6.5 Mon 10:45 POT 81

On the Dynamics of Excitons in Perovskite Nanoplatelets — •Alexander F. Richter[1,2], Verena A. Hintermayr[1,2], Florian Ehrat[1,2], Bernhard Bohn[1,2], Thomas Simon[1,2], Lakshminarayana Polavarapu[1,2], Alexander S. Urban[1,2], and Jochen Feldmann[1,2] — [1]Chair of Photonics and Optoelectronics, Department of Physics and Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität München (LMU), Amalienstraße 54, 80799 Munich, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 Munich, Germany

Organic-inorganic halide perovskites have received great attention in the past few years due to their remarkably high solar energy conversion efficiency. Their functionality is even more widespread showing vast improvements in light-emitting applications, especially in the form of nanocrystals. We have successfully synthesized two-dimensional perovskite nanoplatelets with a controllable thickness down to a single unit cell. This leads to exciton binding energies in the hundred meV range. Here, we present experimental results on the dynamics of excitons in such nanoplatelets. Time-resolved photoluminescence reveals an increased exciton recombination rate with decreasing crystal thickness. In addition, we derive exciton-phonon scattering rates from a linewidth analysis of linear optical spectra. These results are compared to exciton dephasing rates obtained by transient four-wave-mixing experiments.

Coffee break

Invited Talk TT 6.6 Mon 11:30 POT 81

Excitons in ultra-thin perovskites & van der Waals crystals — •Alexey Chernikov — Department of Physics, University of Regensburg, Germany

Excitons, as first introduced by J. Frenkel in 1931, are fundamental quasiparticles in semiconductors, composed from an excited electron and the remaining hole with an effective positive charge bound together by the Coulomb interaction. The excitons strongly influence the materials‘ response to external fields and perturbations, and are of particular importance for a variety of applications, including solar cells, light emitters, lasers, modulators, and detectors. In addition, they play a major role in more advanced concepts, such as entangled photons from biexciton sources, excitonic qubits, carrier multiplication, and Bose-Einstein condensation.

In this talk, I will focus on the properties of excitonic particles in nanostructured two-dimensional materials: single layers of semiconducting organic-inorganic perovskites and van der Waals crystals as thin as a single unit cell. I will discuss the nature of an unusually strong and unconventional Coulomb interaction shared by these systems and demonstrate how it results in exciton binding energies as large as 0.5 eV with highly efficient light-matter interaction, largely determining the optical response of these ultra-thin layers. Finally, I will outline how the excitons can be externally tuned either by electrical and optical injection of charge carriers or through the dielectric engineering of the environment in heterostructures.

TT 6.7 Mon 12:00 POT 81

Carrier dynamics in MoS2 — •Michael Lorke, A. Steinhoff, M. Florian, C. Gies, M. Roesner, T. Wehling, and F. Jahnke — Institute for Theoretical Physics, University of Bremen, Germany

In the context of the current interest in transition-metal dichalcogenides, we study the optical generation and relaxation of excited carriers and their influence on optical properties. In these two-dimensional atomically thin semiconductors, the Coulomb interaction is known to be much stronger than in quantum wells of conventional semiconductors like GaAs, as witnessed by the up to 50 times larger exciton binding energy. The question arises, whether this translates into equivalently faster carrier-carrier Coulomb scattering of excited carriers. We answer this question by combining ab-initio band-structures and single-particle wave functions with kinetic equations for the Coulomb-induced carrier scattering in the full Brillouin zone, We find an ultrafast redistrubution of carriers into different valleys of the band structure on a 100fs timescale. The other main source of carrier relaxation is the interaction of the excited carriers with phonons. To analyze carrier-phonon scattering and dephasing, we solve kinetic equations, based on ab-initio carrier-phonon interaction matrix elements, both for carriers and phonons, including heating effects due to the excitation of non-equilibrium phonons. We find that within 100fs the electrons have relaxed into the valleys of the bandstructure, demostrating fast carrier dynamics, which is accompanied by the generation of non-equilibrium phonons. This process is followed by carrier cooling on a timescale of about 1ps, which is consistent with recent experimental findings.

TT 6.8 Mon 12:15 POT 81

Optical Properties of WSe_2 monolayers on metal films — •Laxmi Narayan Tripathi, Oliver Iff, Simon Betzold, Sven Hoefling, and Christian Schneider — Technische Physik and Wilhelm-Conrad-Roentgen Research Center for Complex Material Systems, Universitaet Wuerzburg, Wuerzburg, Am Hubland, D-97074 Germany

Single photon generation is essential for quantum communications. For efficient quantum communication devices, a core requirement are single photon sources which are stable, bright, and which can be replicated. Recently, quantum light emission from inorganic two dimensional layers of transition metal dichalcogenides (TMDC), such as WSe_2, has been demonstrated.

In this contribution, we present our spectroscopy results from a metal-TMDC hybrid device. We performed low temperature (5K) photoluminescence measurement on a WSe_2 monolayer transferred mechanically on metal surface and obtained stable and sharp emission features as compared to bare TMDC monolayer on dielectric substrate. The nanoscale metal surface sample were prepared in the group of Prof Dai-Sik Kim, Seoul National University, South Korea. We envisage that the results will find application in quantum photonics.

TT 6.9 Mon 12:30 POT 81

Tamm-Plasmon Exciton-Polaritons with a WS2 monolayers at room temperature — •Sebastian Stoll[1], Nils Lundt[1], Christian Schneider[1], and Sven Höfling[1,2] — [1]Technische Physik and Wilhlem-Conrad-Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Am Hubland, Germany — [2]SUPA, School of Physics and Astronomy, University of St. Andrews KY 16 9SS, UK

We demonstrate the formation of room temperature Tamm-plasmon Exciton-polaritons with a WS2 monolayer. Due to their high oscillator strength and stable excitonic complexes at 300 K, transition metal dichalcogenide monolayers have awaken strong interest in the field of light-matter interaction at high temperatures. Recently, WS2 was brought into the strong coupling regime by embedding it into both an open-cavity [1] and a Fabry-Perot-cavity consisting of two silver mirrors [2]. In this experiment, the use of a Tamm structure provides us with a narrower cavity linewidth and thus with a higher cavity Q-factor. The exciton-polariton dispersion was measured by momentum-resolved PL spectroscopy. The acquired dispersion shows the expected avoided crossing behaviour of the two polariton branches and yields a Rabi splitting of around 27 meV. References: [1] L.C. Flatten et al., Scientific Reports 6, 33134 (2016) [2] S. Wang et al., Nano Letters 16, 7 (2016)

TT 7: Spintronics I (joint session DS, HL, MA, TT, organized by HL)

Time: Monday 9:30–13:00 Location: POT 151

TT 7.1 Mon 9:30 POT 151

Dynamical spin-orbit-based spin transistor — •Fahriye Nur Gürsoy[1,2], Phillipp Reck[1], Cosimo Gorini[1], Klaus Richter[1], and Inanç Adagideli[2] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Faculty of Engineering and Natural Sciences, Sabanci University, Orhanli-Tuzla, Istanbul, Turkey

Spin-based devices are highly important for the future of information technology. In this project we focus on a mesoscopic 2-Dimensional Electron Gas (2DEG) with time-dependent Rashba spin-orbit interaction, which can be engineered via an AC top gate.

Spin-orbit coupling in 2DEGs can be rewritten in terms of appropriate SU(2) gauge fields, so as to clearly identify the relevant Onsager symmetries [1, 2].The latter can then be exploited for the realisation of spin transistor devices, in particular when the spin-orbit interaction is non-homogeneous through the sample [1]. On the other hand, a dynamical Rashba interaction was suggested as a generator of spin-motive forces. Here we merge the two concepts, and explore the possibilities of realising a spin transistor in a quantum coherent sample driven by a time-dependent Rashba field. We follow a mixed analytical-numerical approach, and compute the (spin) conductance and the pumping (spin) current of the periodically driven system with the Floquet Hamiltonian method [3].

[1] I. Adagideli, et al., Phys. Rev. Lett. 108, 236601 (2012).
[2] C. Gorini, et al., Phys. Rev. Lett. 109, 246604 (2012).
[3] J. H. Shirley, Phys. Rev. 138, B979 (1965).

TT 7.2 Mon 9:45 POT 151

Coherent electron Zitterbewegung triggered by ps optical pulses — •Manfred Ersfeld[1], Ivan Stepanov[1], Alexander V. Poshakinskiy[2], Mihail Lepsa[3], Eugeneous L. Ivchenko[2], Sergey A. Tarasenko[2], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, D-52074 Aachen, Germany — [2]Ioffe Institute, 194021 St Petersburg, Russia — [3]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich GmbH, Germany

Zitterbewegung is a direct consequence of relativistic quantum mechanics which predicts that free Dirac electrons exhibit a rapid trembling motion even in the absence of external forces. Recent theoretical studies have shown that electrons in III-V semiconductors also exhibit

Zitterbewegung caused by the spin orbit interaction. Here we probe the Zitterbewegung of electrons in n-type InGaAs as an AC electric current. We trigger the coherent electron Zitterbewegung by optical initialization of an ensemble of electron spins in the same spin states and control the frequency of electron oscillations in real space by tuning the Larmor spin precession frequency in an external magnetic field.

TT 7.3 Mon 10:00 POT 151

On the link between charge- and spin-dynamics in PBTTT — •Uday Chopra[1], Erik R. McNellis[1], Denis Andrienko[2], Pascal Kordt[2], and Jairo Sinova[1] — [1]Johannes Gutenberg University, Mainz, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany

In the nascent field of organic spintronics, charge- and spin-dynamics are strongly linked. We study this relationship in a high-mobility[1], spin-conducting polymer[2], PBTTT, using a newly developed multi-scale modelling framework. High mobility ($\sim$ 1 $cm^2V^{-1}s^{-1}$) in PBTTT along the $\pi-\pi$ stacking direction is attributed to its highly ordered structure and hence the strong transfer integrals in the same direction. However, the mechanism for spin transport and its correlation with electron transport is still unclear. We demonstrate the anisotropy in electron dynamics of PBTTT by calculating electron transfer rates for morphologies of different sizes and extent of disorder in the backbone using Marcus theory and Kinetic Monte Carlo (KMC) as implemented in VOTCA-CTP[3] and showing the field and temperature dependence of mobility along different crystalline axes. In addition to it, we present an approach for spin transport in organic semiconductors build on top of VOTCA-CTP via first-principles modelling of spin relaxation mechanisms which allows us an uprecedented insight into the explicit dependence of spin- on charge-dynamics and the parameters that correlate them. [1] McCulloch et al., Nat. Mater., 2006, 5, 328. [2] Watanabe et al., Nat. Phys., 2014, 10, 308. [3] V. Rühle et al. J Chem. Theory Comput., 2011, 7, 3335.

TT 7.4 Mon 10:15 POT 151

Theory of current-induced spin polarisations in a 2DEG — Amin Maleki[1], •Cosimo Gorini[2], Ka Shen[3], Ilya V. Tokatly[4,5], Giovanni Vignale[6], and Roberto Raimondi[1] — [1]CNISM e Dipartimento di Fisica, Università Roma Tre, Rome, Italy — [2]Institut für Theoretische Physik, Universität Regensburg, Regensburg, Germany — [3]Kavli Institute of NanoScience, Delft University of Technology, Delft, Netherlands — [4]Nano-Bio Spectroscopy group, Dpto. Fisica de Materiales, Universidad del País Vasco, San Sebastián, Spain — [5]IKERBASQUE, Bilbao, Spain — [6]Department of Physics and Astronomy, University of Missouri, Columbia, Missouri, USA

The Bloch equations for the spin dynamics of a 2DEG are derived in the presence of intrinsic (Rashba and Dresselhaus) and extrinsic (impurities) spin-orbit coupling. In comparison to previous analyses, we find new terms arising from the interplay between the two types of spin-orbit interaction. These influence current-induced spin polarisations (CISP), which are shown to have a more complex symmetry with respect to that of the internal Rashba-Dresselhaus field. Our results are derived both diagrammatically and via a semi/quasi-classical approach, based on a SU(2) gauge formulation of spin-orbit coupling.

TT 7.5 Mon 10:30 POT 151

Toward accurate calculation of diffusive spin transport starting from realistic Hamiltonians. Applications to electrons, excitons, and topological insulators. — •Vincent Sacksteder[1] and Yasufumi Araki[2] — [1]W155 Wilson Building, Royal Holloway University of London, Egham Hill, Egham, TW20 0EX, United Kingdom — [2]Creative Interdisciplinary Research Division, Tohoku University

Spin-orbit couplings, in the presence of an electric current, can generate strong spin currents with possible applications to magnetic domain switching in new memory devices. This talk will focus on a coarse-graining strategy which starts from realistic Hamiltonians describing spin and scattering at the atomic scale, and derives spin diffusion equations suitable for modeling a spintronics device. After reviewing the standard formalism, we outline how spin diffusion coefficients can be calculated either analytically or numerically, in either magnetized or unmagnetized systems. We present results for spin lifetimes, spin polarization production, and characteristic spatial patterns in electron gases, excitons, and topological insulators.

TT 7.6 Mon 10:45 POT 151

Charge- and Spin Dynamics in Organic Spintronics from First-Principles Theory: VOTCA-STP — •Erik R. McNellis[1], Shayan Hemmatiyan[1,2], Amaury Melo Souza[1], Sebastian Müller[1], Sergei A. Egorov[1,3], Denis Andrienko[4], and Jairo Sinova[1] — [1]Johannes Gutenberg University, Mainz, Germany — [2]Texas A & M University, College Station, USA — [3]University of Virginia, Charlottesville, USA — [4]Max-Planck-Institute for Polymer Research, Mainz, Germany

Novel high-mobility materials based on organic molecules bring a host of advantages in spintronic applications. In organics, spin- and charge dynamics are intimately linked. Ideally, such materials should be theoretically modeled using realistic structural models with atomic resolution, and field- and spin-orbit coupling (SOC) effects calculated from state-of-the-art first-principles theory.

We present a multi-scale framework for modeling of spin-dynamics in organics, implemented on top of the electron dynamics given by the VOTCA-CTP package[1]. This development allows us to accurately treat the balance of SOC phenomena in realistic morphologies, while observing the link between charge- and spin-dynamics directly.

Our results include a complete map of the spin-relaxation in Alq_3 - the organic spintronics fruit-fly - as a function of charge concentration and temperature. Additionally, insights into the highly spin conducting polymer PBTTT will be presented, along with developments towards treating the spin Hall and Nernst effects.

1. V. Rühle et al., J Chem. Theory Comput. **7**, 3335 (2011)

Coffee Break

TT 7.7 Mon 11:30 POT 151

Control of spin helix symmetry in semiconductor quantum wells by crystal orientation — •Paul Wenk, Michael Kammermeier, and John Schliemann — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We investigate the possibility of spin-preserving symmetries due to the interplay of Rashba and Dresselhaus spin-orbit coupling in n-doped zinc-blende semiconductor quantum wells of general crystal orientation. It is shown that a conserved spin operator can be realized if and only if at least two growth-direction Miller indices agree in modulus. We determine the appropriate requirements on the axial symmetric Rashba and Dresselhaus contributions and discuss the impact of cubic Dresselhaus terms which break this symmetry. We observe that including the latter commonly inhibits a perfect realization of the persistent spin helix symmetry except for two specific directions, i.e., [110] and [111]. Furthermore, by analyzing the spectrum of the spin diffusion equation, we show that besides the cases of perfect spin-preserving symmetries, the spin of the long-lived homogeneous spin state relaxes about a factor 2 faster than for the helical spin state. To support experimental probing, we additionally provide analytical expressions for the weak (anti)localization correction and the characteristic shift of the magnetoconductivity minima [2] which show an imprint of the peculiar symmetry.

[1] M. Kammermeier *et al.*, Phys. Rev. Lett. **117**, 236801 (2016)
[2] K. Yoshizumi *et al.*, Appl. Phys. Lett. **108**, 132402 (2016).

TT 7.8 Mon 11:45 POT 151

Hidden orbital polarization in centrosymmetric materials — •Ji Hoon Ryoo and Cheol-Hwan Park — Department of Physics & Astronomy, Seoul National University 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Korea

Until recently, the possibility of spatial spin distribution in centrosymmetric and non-magnetic materials was largely dismissed, because their electronic bands are degenerate even if spin-orbit coupling is strong. However, Zhang et al. [1] has pointed out that even in those materials, the degenerate Bloch states can have spin polarization localized at different sites in real space, significantly broadening the scope of spintronics to materials with inversion symmetry. On the other hand, the orbital magnetic moment could play as an important role as the spin moment in the magnetization of solids, in both equilibrium and non-equilibrium situations [2-5]. In this talk, we report that the hidden, or sublattice-dependent orbital polarization of Bloch states can be large in common centrosymmetric materials, and suggest some implications of this finding to photoemission spectroscopies and antiferromagnetic information technology.

1. X. Zhang et al., Nat. Phys. 10, 387 (2014).
2. R. A. Reck and D. L. Fry, Phys. Rev. 184, 492 (1969).
3. D. Ceresoli et al., Phys. Rev. B 81, 060409 (2010).
4. T. Yoda, T. Yokoyama, and S. Murakami, Sci. Rep. 5, 12024

(2015).
5. S. Zhong, J. E. Moore, and I. Souza, Phys. Rev. Lett. 116, 077201 (2016).

TT 7.9 Mon 12:00 POT 151

Improving and tailoring the magnetic properties of thin Fe layers by making use of exchange coupling — •Markus Ehlert, Helmut Körner, Thomas Hupfauer, Markus Schitko, Christian Back, Günther Bayreuther, and Dieter Weiss — Institute of Experimental and Applied Physics, University of Regensburg, Germany

The control of the magnetic properties of thin ferromagnetic films is crucial for the functionality of spintronic devices, e.g., for the detection of the spin Hall effect [1]. The goal of our work is to improve the magnetic stability of commonly used Fe layers by making use of the exchange coupling between soft magnetic Fe and hard magnetic Dysprosium (Dy). Microstructured thin films of Fe, Dy, and Fe-Dy multilayers were prepared by electron-beam lithography and ultra-high vacuum sputtering. The magnetic properties of the materials were determined by means of the AMR effect. By analyzing and comparing the corresponding AMR data we show that the presence of a Dy layer on top of the Fe layer significantly influences and enhances the magnetic properties of the Fe layer. We also investigated the temperature dependence of this effect and its dependence on the thickness of the Fe layer. All experimental results can consistently be explained with the model of the AMR effect and are also confirmed by corresponding SQUID measurements of full film samples.

[1] M. Ehlert *et al.*, Phys. Status Solidi B **251**, 1725-1735 (2014).

TT 7.10 Mon 12:15 POT 151

First principles calculations to address key spin relaxation mechanisms in organic semiconductors — •Amaury de Melo Souza[1], Sergei Ergorov[2], Pedro Brandimarte[3], Sebastian Mueller[1], Uday Chopra[1], Shayan Hemmatiyan[4], Denis Andrienko[5], Ilja Mueller[1], Jairo Sinova[1], and Erik McNellis[1] — [1]Johannez Gutenberg University, Mainz, Germany — [2]University of Virginia, Charlottesville, USA — [3]University del Pais Vasco, San Sebastian, Spain — [4]Texas A&M University, College Station, USA — [5]Max Planck Institute for Polymers, Mainz, Germany

In this work, we present our theoretical framework to simulate simultaneously spin and charge transport in amorphous organic semiconductors. By combining several techniques e.g. molecular dynamics, density functional theory and kinetic Monte Carlo, we are able to study spin transport in the presence of anisotropy, thermal effects, magnetic and electric field effects in realistic morphologies of amorphous organic systems. In this talk, we present in detail first-principles calculations combined with perturbation theory in order to extract the relevant quantities required to address key spin relaxation mechanisms, namely, spin flip due to spin-orbit coupling, intra-site spin relaxation due to spin-orbit coupling and electron-phonon coupling and exchange mediated transport. Finally, we apply our approach to a realistic morphology of Alq3 (Tris(8-hydroxyquinolinato)aluminum) and identify which spin relaxation mechanism is dominant in this system.

Invited Talk TT 7.11 Mon 12:30 POT 151

Carbon nanotubes as excitonic insulators — •Massimo Rontani — CNR-NANO, Modena, Italy

Fifty years ago Walter Kohn speculated that a zero-gap semiconductor might be unstable against the spontaneous generation of excitons—electron-hole pairs bound together by Coulomb attraction. The reconstructed ground state would then open a gap breaking the symmetry of the underlying lattice, a genuine consequence of electronic correlations.

I will show that this 'excitonic insulator' is realized in zero-gap carbon nanotubes, by presenting results of first-principles calculations performed by means of many-body perturbation theory as well as quantum Monte Carlo. The excitonic order modulates the charge between the two carbon sublattices of the armchair tube, opening an experimentally observable gap which scales as the inverse of the tube radius and weakly depends on the axial magnetic field.

These findings invalidate the common wisdom that the ground state of armchair carbon nanotubes is a Luttinger liquid. I will discuss the physical origin of this conclusion, related to the strong e-h binding in quasi-1D and the almost unscreened long-range interactions in undoped nanotubes. Finally, I will propose independent experimental tests to discriminate between the excitonic insulator and the Luttinger liquid at strong coupling (Mott insulator).

This work is performed together with Daniele Varsano, Sandro Sorella, Davide Sangalli, Matteo Barborini, Stefano Corni, and Elisa Molinari.

TT 8: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - I (joint session DS, HL, MA, MM, O, TT, organized by O)

Time: Monday 10:30–13:00 Location: GER 38

TT 8.1 Mon 10:30 GER 38

DFT wants U: Embedded-cluster calculations of surface oxygen vacancies at TiO_2 with Hubbard-corrected DFT — •Matthias Kick, Karsten Reuter, and Harald Oberhofer — Technische Universität München

Surface oxygen vacancies, in particular their nature as charge trapping centers, play an inportant role for many oxide materials properties. However, addressing them with first-principles density-functional theory (DFT) computations remains a challenge. At least Hubbard corrected DFT+U is required to achieve an appropriate electron localization. At the same time, the large dielectric constant of polarizable oxides like TiO_2 leads to a strong polarization response. As a result supercells of increasing size are necessary in order to avoid spurious interactions between periodic images in case of charged defects, rendering the conventional periodic boundary condition supercell approach impractical.

Full DFT+U functionality has been implemented in the all-electron electronic structure code FHI-aims. Combined with the solid state (QM/MM) embedding functionality in FHI-aims, this yields a numerically most efficient approach to treat aperiodic aspects at oxide surfaces. We illustrate this by calculating neutral and charged states of the surface oxygen vacancy at rutile TiO_2 (110). We systematically assess the reliability and computational efficiency by comparing to hybrid-level DFT calculations and calculations performed in conventional supercells.

TT 8.2 Mon 10:45 GER 38

Hubbard interactions from density-functional perturbation theory — •Iurii Timrov, Matteo Cococcioni, and Nicola Marzari — Theory and Simulation of Materials (THEOS), and NCCR-MARVEL, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

DFT+U, together with its V and J extensions, is a simple and powerful tool to model systems containing partially-filled manifolds of localized states [1]. However, the Hubbard parameters are often - and in our view incorrectly - treated semi-empirically. Conceptual and practical methods to determine e.g. the Hubbard U parameter have nevertheless been introduced long ago, based either on the constrained random-phase approximation (cRPA) or on linear-response theory [2]. These approaches make DFT+U a fully first-principles and self-contained method, but are often overlooked due to their cost or complexity. Here, we introduce a computationally inexpensive and straightforward approach to determine the linear-response U, hitherto obtained from the difference between bare and self-consistent inverse electronic susceptibilities evaluated from supercell calculations. By recasting these calculations in the language of density-functional perturbation theory we remove the need of supercells, and allow for a fully automated determination of susceptibilities and Hubbard parameters. Such developments open the way for deployment in high-throughput studies, while providing the community with a simple tool to calculate consistent values of U for any system at hand. [1] V. Anisimov et al., PRB 44, 943 (1991), [2] M. Cococcioni et al., PRB 71, 035105 (2005).

TT 8.3 Mon 11:00 GER 38

Time-evolution using full configuration interaction quantum Monte Carlo — •Kai Guther[1], Werner Dobrautz[1], Olle

Gunnarsson[1], and Ali Alavi[1,2] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, United Kingdom

We report on a new method to perform real-time quantum evolution of a fermionic system using the full configuration interaction quantum Monte Carlo method [1]. To stabilize the algorithm, a slow simultaneous imaginary-time evolution is performed, yielding properties for times slightly rotated into the complex plane.

We employ this technique to compute Green's functions and therefore by means of analytic continuation also spectral weight functions. We demonstrate the applicability of the algorithm using the examples of the 2D-Hubbard model and the carbon dimer, showing that the algorithm can in principle be used as an Anderson solver for DMFT and is capable of obtaining photoemission spectra of ab-initio systems.

[1] G.H. Booth, A.J.W. Thom and A. Alavi, J. Chem. Phys. 131, 054106 (2009)

TT 8.4 Mon 11:15 GER 38

Laplace-transformed MP2 with localized Resolution of Identity for molecular and periodic systems — •Arvid Ihrig, Igor Ying Zhang, and Matthias Scheffler — Fritz-Haber-Institut, Berlin, Germany

The self-interaction error is a well-known problem in (semi)local functionals in density-functional theory (DFT) and to a lesser extend also in hybrid functionals. It leads to a quantitatively and sometimes even qualitatively wrong description. One possible remedy is the 2nd order Moller-Plesset perturbation theory (MP2) and the double-hybrid DFT methods based on it. However, the time and memory requirements prevent their routine-usage for large molecular and condensed-matter systems.

In this work we combine our localized Resolution of Identity (RI-LVL) [1] and its favourable memory requirements with the low-order scaling of the Laplace-transformed MP2 (LT-MP2) [2]. Our highly parallelizable LT-MP2 implementation in a numeric atom-centered orbital (NAO) framework allows us to treat both cluster and periodic models in the same computational environment. We demonstrate the accuracy and other features of our implementation for examples of water clusters and TiO_2 surfaces with small absorbed molecules. We furthermore present a way how the distance-dependent integral screening [3] from the Ochsenfeld group can be generalized to periodic systems.

[1] Ihrig et al., New J. Phys. 17, 093020 (2015)
[2] P. Ayala et al., J. Chem. Phys. 110, 3660 (1999)
[3] S. Maurer et al., J. Chem. Phys. 136, 144107 (2012)

TT 8.5 Mon 11:30 GER 38

Bond Disproportionation in Rare-Earth Nickelates: Describing Lattice Distortions within DFT+DMFT — •Alexander Hampel and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

Perovskite rare-earth nickelates, $R\mathrm{NiO}_3$, display a rich and only partially understood phase diagram, where all compounds with R from Pr to Lu undergo a metal-insulator transition (MIT), that is accompanied by a structural distortion. This distortion breaks the symmetry between formerly equivalent Ni sites and can (in the simplest picture) be understood as a charge disproportionation of the Ni^{3+} cations into Ni^{2+} and Ni^{4+}. Here, we use density functional theory (DFT) and its extensions (DFT+U, DFT+DMFT) combined with symmetry-based distortion mode analysis to explore the interplay between lattice distortions, magnetic order and electronic correlation effects in rare-earth nickelates. Thereby, we want to explore the capabilities of the DFT+DMFT method to describe complex materials with coupled electronic and structural degrees of freedom by comparing with DFT+U results and available experimental data.

TT 8.6 Mon 11:45 GER 38

Density matrix embedding theory for coupled fermion-boson systems — •Teresa E. Reinhard[1], Uliana Mordovina[1], Heiko Appel[1], Joshua S. Kretchmer[2], Garnet K. L. Chan[2], and Angel Rubio[1,3] — [1]Max Planck Institut für Struktur und Dynamik der Materie, Hamburg — [2]Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian

We analyze strongly correlated fermion-boson systems by extending Density Matrix Embedding Theory (DMET) from the purely electronic case [1] to coupled fermion-boson systems. DMET is a novel embedding theory which uses the Schmidt decomposition to divide the treated system into an impurity and a bath part. We project the bath part into the part of the Fock space that contains the entanglement with the impurity region and then solve this much smaller entangled system with exact diagonalization and DMRG.

With this technique, we treat lattice systems of Hubbard-Holstein type, where fermions and bosons are coupled by a bilinear Froehlich coupling. As we choose coherent states for the bosonic basis set, it is convenient to apply our approach to electron-phonon as well as to electron-photon systems.

By using a DMRG solver for the DMET algorithm, an accurate treatment of 2 dimensional systems becomes feasible.

[1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012)

TT 8.7 Mon 12:00 GER 38

Vertex function of homogeneous electron gas — •Yaroslav Pavlyukh — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, P.O. Box 3049, 67653 Kaiserslautern, Germany — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

We present a systematic study of the vertex function correction in homogeneous electron gas at metallic densities [1]. Contrary to a popular belief the vertex function not only provides corrections to the well known plasmon or particle-hole pair scatterings, but also gives rise to new physical processes such as generation of two plasmon excitations or the transformation of the initial one-particle state into a two-particles-one-hole state. Using a merger of the many-body perturbation and scattering theories, which is a distinct feature of our method, it is shown that additional scattering channels are responsible for the bandwidth reduction (as observed in photoemission experiments on bulk sodium), appearance of the secondary plasmonic satellite below the Fermi level and lead to a substantial modification of the electron spectral function.

[1] Y. Pavlyukh, A.-M. Uimonen, G. Stefanucci, R. van Leeuwen, Phys. Rev. Lett. **117**, 206402 (2016)

TT 8.8 Mon 12:15 GER 38

Coupled-Cluster approaches for molecules and solids in the numeric atom-center orbital framework — •Tonghao Shen, Igor Ying Zhang, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, DE

As a well-established and successful wave-function theory hierarchy in quantum chemistry, the coupled-cluster (CC) ansatz is attracting increasing attention in computational materials science [1]. However, compared to traditional density-functional approximations, CC approaches face much greater challenges regarding numerical implementation, bassis-set accuracy and efficiency, in particular for solids [2]. In this report, we present a highly parallel implementation of the CC approaches with singles, doubles and perturbative triples, CCSD(T), in the numeric atom-center orbital (NAO) framework. This implementation allows CCSD(T) simulations to be carried out using both cluster and periodic models in a single computational environment. Taking some popular quantum-chemistry test sets (S22, ISO34, and CYCONF), we demonstrate that CCSD(T) with correlation-consistent NAO basis sets [3] can provide accurate reference data for molecular properties. Our solid-state examples include elemental and binary crystals, as Ne (fcc), C, Si (diamond), LiF, MgO (rocksalt), and BN (zincblende).

TT 8.9 Mon 12:30 GER 38

Implementation of the SU(2) Symmetry in FCIQMC using the Graphical Unitary Group Approach — •Werner Dobrautz[1] and Ali Alavi[1,2] — [1]Max-Planck-Institut für Festkörperforschung — [2]Department of Chemistry, University of Cambridge

The Full Configuration Interaction Quantum Monte Carlo (FCIQMC) algorithm [1] is a projector QMC method, previously formulated in the total anti-symmetric space of Slater Determinants, based on the imaginary-time Schrödinger equation to obtain the ground state of a system in the long-time limit.

By formulating the method in eigenfunctions of the $\hat{S}^2$ spin-operator via the Graphical Unitary Group Approach [2] we can make use of the block-diagonal form of spin-preserving, non-relativistic Hamiltonians for different values of the total spin. This allows us to lift possible near degeneracies of low-lying excitations of different spin sectors, calculate spin-gaps more easily and obtain the physical correct ground-state, without spin-contamination, and identify its total spin quantum number.

Our method does not rely on expanding the spin-eigenfunctions in linear combinations of Slater Determinants and thus does not hit an exponential bottle neck and can be applied to system sizes larger than previously reachable with similar approaches.

[1] G. Booth, A. Thom and A. Alavi, J. Chem. Phys. **131**, 054106 (2009)
[2] I. Shavitt, Int. J. Quantum Chem. Symp., **11:** 131 (1977); Int. J. Quantum Chem. Symp., **12:** 5 (1978)

TT 8.10 Mon 12:45 GER 38

A study of the dense uniform electron gas with high orders of coupled cluster — •Verena Andrea Neufeld and Alex James William Thom — University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, United Kingdom

We used the recently developed stochastic coupled cluster method [Phys. Rev. Lett. (2010) 105, 263004 and J. Chem. Phys. (2016) 144, 084108] to benchmark the dense uniform electron gas (UEG). The aim was to make predictions about what truncation level of coupled cluster is needed to reach sufficient accuracy in electronic correlation energies for a range of electron densities. This will aid our future studies of solids with stochastic coupled cluster.

We take advantage of sparsity in wavefunctions by doing coupled cluster stochastically. In this study, we used coupled cluster truncation levels up to CCSDTQ5, that includes single, double, triple, quadruple and quintuple excitations directly. We considered the 14 electron UEG with Wigner-Seitz radius in the range 0.5 to 5.0 a.u.. We applied coupled cluster truncations from CCSD to CCSDTQ5 and extrapolated to the complete basis set size limit. By comparing the differences in energy calculated with CCSD to CCSDTQ5, we learn what truncation level is necessary for sufficient accuracy. What truncation level is needed, is dependent on the level of correlation, which decreases with electron density. We are therefore able to relate the degree of correlation linked to electron density to the level of coupled cluster needed for accuracy. This information will prove valuable when tackling periodic solids that can be approximated by the UEG.

TT 9: Focus Session: Two-Dimensional Materials II (joint session DS, HL, TT, organized by HL)

Time: Monday 14:45–18:15 Location: POT 81

Invited Talk TT 9.1 Mon 14:45 POT 81

2D / 3D Heterostructures for Optoelectronis — •Max Lemme — University of Siegen, Germany

Broad spectral optical detection is of high interest for imaging, sensing, communication and spectroscopy. Two-dimensional (2D) materials are very promising for such applications due to their high optical absorption, potential wide detection range and material flexibility.

In this talk, graphene / silicon Schottky diodes made of chemical vapor deposited (CVD) graphene on n-type Si substrates will be discussed. Broad spectral response of 60 - 407 mA/W is measured from ultraviolet to near infrared light. In contrast to graphene, bulk molybdenum disulfide (MoS_2) is an n-type semiconducting 2D material with an indirect band gap of 1.3 eV. MoS_2/Si hybrid diodes made with multilayer, CVD grown MoS_2 yield a maximum spectral response of 8.6 mA/W.

Hybrid integration of large area CVD graphene as transparent conductive electrodes with amorphous silicon (a-Si) will be discussed for applications as multispectral photodetectors. A strong enhancement of the detectors' spectral response is observed in the ultraviolet region compared to reference devices with conventional aluminum doped zinc oxide electrodes. The maximum responsivity of these multispectral PDs can be tuned in their wavelength from 320 nm to 510 nm by external biasing, which allows single pixel detection of UV to visible light. The material combination of graphene and a-Si enables flexible diodes on polyimide substrates. Bilayer graphene boosts the maximum photoresponsivity of these flexible diodes up to 239 mA/W.

TT 9.2 Mon 15:15 POT 81

Optical properties of atomically thin MoS2 exposed to helium ions — •Anna Nolinder[1], Julian Klein[1,2], Agnieszka Kuc[4], Marcus Altzschner[1], Jakob Wierzbowski[1], Florian Sigger[1], Franz Kreupl[3], Thomas Heine[4], Jonathan Finley[1,2], Ursula Wurstbauer[1,2], Alexander Holleitner[1,2], and Michael Kaniber[1] — [1]Walter Schottky Institut und Physik Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 München, Germany — [3]Department of Hybrid Electronic Systems, Technische Universität München, Arcisstr. 21, 80333 Munich, Germany — [4]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstr. 2, 04103 Leipzig, Germany

We present a spectroscopic study on atomically thin MoS2 exposed to helium ions. Distinct changes of the first-order Raman bands, additional defect luminescence and strong modification of the intrinsic valley spin relaxation properties are observed, shedding light on the effect of disorder on the optical properties and valley spin relaxation mechanisms. Moreover, our observations are in good qualitative agreement with Density Functional Theory calculations.

TT 9.3 Mon 15:30 POT 81

Coulomb Engineering of Excitonic Transitions in Transition Metal Dichalcogenides for New Non-Classical Light Sources — •Sven Borghardt[1], Jhih-Sian Tu[1], Tim Flatten[2], Frank Matthes[2], Daniel Bürgler[2], Detlev Grützmacher[1], and Beata Kardynal[1] — [1]Peter Grünberg Institute 9 (PGI-9), Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Peter Grünberg Institute 6 (PGI-6), Forschungszentrum Jülich, D-52425 Jülich, Germany

The spatial confinement of excitons is a key prerequisite for the creation of non-classical light sources. Since the dielectric environment of transition metal dichalcogenide monolayers (TMD-MLs) changes the screening of electrostatic fields and, thus, the interaction of charge carriers within the MLs, both the single particle band gap and the binding energy of exciton complexes in TMD-MLs can be tuned by modifying the dielectric properties of the environment.

In our experiments, we prepare TMD-MLs in different environments and apply optical spectroscopy methods in order to quantify the effects of the dielectric environment on the transition energies of exciton complexes. Furthermore, we correlate the results with single particle band gaps estimated from excited exciton states and single particle band gaps measured in scanning tunnelling spectroscopy experiments. This correlation gives access to the binding energy of exciton complexes.

In addition to TMD-MLs in laterally homogeneous environments, we examine lateral heterostructures of TMD-MLs in environments with laterally changing dielectric properties, paving the way towards controllable confinement of excitons within TMD-MLs.

TT 9.4 Mon 15:45 POT 81

Exciton-trion competition and single photon emission in III-V- monolayer hybrid architectures — •Oliver Iff[1], Yu-Ming He[1], Nils Lundt[1], Sebastian Stoll[1], Vasilij Baumann[1], Sven Hoefling[1,2], and Christian Schneider[1] — [1]Technische Physik and Wilhelm Conrad Roentgen Research Center for Complex Material Systems, Physikalisches Institut, Universitaet Wuerzburg, Am Hubland, D-97074 Wuerzburg, Germany — [2]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

Atomic monolayers represent a novel class of materials to study localized and free excitons in two dimensions and to engineer optoelectronic devices based on their significant optical features. Here, we investigate the role of epitaxially grown III-V substrates on the photoluminescense response from exfoliated MoSe2 and WSe2 monolayers in comparison to regular SiO2 substrates. In the case of MoSe2, we observe a significant qualitative modification of the emission spectrum, which is widely dominated by the trion resonance on InGaP substrates. Even more remarkably, in sheets of WSe2, we notice emission lines from localized excitons with linewidths down to 70 μeV, only limited by our system resolution. Furthermore, these spectral signatures are identified as single photon or even photon pair emitters without any sign of spectral jitter or blinking. Overall, the results outline the enormous potential of hybrid III-V- monolayer architectures in obtaining high quality emission signals from atomic monolayers, enhancing their

optical properties.

TT 9.5 Mon 16:00 POT 81

The Influence of the Substrate Material on the Optical Properties of Tungsten-Diselendide Monolayers — Sina Lippert[1], •Lorenz Schneider[1], Dylan Renaud[1], Kyung Nam Kang[2], Obafunso Ajayi[3], Marc Halbich[1], Oday Abdulmunem[1], Xing Lin[1], Jan Kuhnert[1], Khaleel Hassoon[1], Saideh Edalati-Boostan[1], Young Duck Kim[3], Wolfram Heimbrodt[1], Eui-Hyeok Yang[2], James Hone[3], and Arash Rahimi-Iman[1] — [1]Faculty of Physics, Philipps-Universität, Marburg 35032, Germany — [2]Department of Mechanical Engineering, Stevens Institue of Technology, Hoboken, New Jersey, 07030, USA — [3]Department of Mechanical Engineering, Columbia University, New York, New York, 10027, USA

In recent years 2D materials based on transition metal dichalogenides (TMDs) have come up as an interesting material system mainly due to their remarkable properties in the monolayer regime after the successful exploration of graphene. While the main optical properties of these materials have been studied and understood well, the influence of the substrate material on the energy levels and the recombination dynamics are not yet sufficiently discussed. Here, we present a systematic comparison of the optical properties of monolayered WSe_2 on different substrates including SiO_2, sapphire, Si_3N_4-hBN and MgF_2. In addition to the exfoliated monolayers, a CVD grown monolayer on sapphire is included. While similarities have been found for the Raman signal and PL of these samples, small differences regarding excitonic features, emission characteristics and decay dynamics have been observed in dependence on the substrate.

Coffee Break

Invited Talk TT 9.6 Mon 16:45 POT 81

Excitons in colloidal 2D-CdSe nanocrystals — •Ulrike Woggon — Institut für Optik und Atomare Physik, TU Berlin, Str. des 17. Juni 135, 10623 Berlin, Germany

Two-dimensional II-VI semiconductor nanoplatelets (NPLs) gained increasing interest because of their unique electronic and optical properties, such as the Giant Oscillator Strength, strong electroabsorption response, low exciton-phonon interaction and high impact of dielectric confinement on exciton binding energies [1]. CdSe platelets are of special importance since they combine large particle volumes with ultrastrong confinement. We present a comprehensive study of the influence of dimensionality, size and shape on excitons in CdSe NPLs. They are an attractive system allowing to control not only the exciton energy states by thickness (z-direction) but also with lateral size variation the LO-phonon coupling (x,y-direction) [2]. The larger the particles' aspect ratio, the greater is the confinement related electronic contribution to the increased two-photon absorption and CdSe NPLs are ideally suited for two-photon imaging and non-linear opto-electronics [3-5]. [1] A.W. Achtstein et al., Nano Letters 12, 3151 (2012); [2] A.W. Achtstein et al., Phys. Rev. Lett. 116, 116802 (2016); [3] A.W. Achtstein et al., J. Phys. Chem. C 119, 20156 (2015); [4] R. Scott et al., Nano Lett. 15, 4985 (2015); [5] A.W. Achtstein et al., ACS Nano 8, 7678 (2014)

TT 9.7 Mon 17:15 POT 81

Controlled MoS2 deposition by metal-organic vapour phase epitaxy — Matthias Marx[1], Dominik Andrzejewski[2], Annika Grundmann[1], You-Ron Lin[1,3], Gerd Bacher[2], Holger Kalisch[1], Andrei Vescan[1], and •Michael Heuken[1,3] — [1]GaN Device Technology, RWTH Aachen University — [2]WET, University Duisburg-Essen — [3]AIXTRON SE

Recently, layered transition metal dichalcogenides (TMDC) have attracted a lot of attention. Their thermodynamically stable 2D form and their unique electrical and optical properties are very promising for integration in future electronic devices. For systematic scientific studies and in particular for implementation in commercial devices, it will be necessary to achieve a reproducible, homogeneous and scalable deposition on wafer scale. A promising option to achieve this goal is to use metal-organic vapour phase epitaxy (MOVPE) processes employing MO precursors for the TMDC constituents. All deposition experiments reported here are carried out in an AIXTRON horizontal hot-wall reactor. Molybdenum hexacarbonyl (MCO) and Di-tert-butyl sulfide (DTBS) are used as Mo and S sources, respectively. The samples are characterized via Raman spectroscopy, photoluminescence (PL) spectroscopy, atomic force microscopy (AFM) and scanning electron microscopy (SEM) to investigate their optical and structural properties. To reduce and control the nucleation density and to promote a layer-by-layer growth mode, the growth parameters such as DTBS and MCO precursor flows are optimized and temperature treatment was adjusted.

TT 9.8 Mon 17:30 POT 81

Ion implantation of 2D transition metal dichalcogenides monolayers — •Jhih-Sian Tu[1], Sven Borghardt[1], Hans Hofsass[2], Ursel Bangert[3], Quentin Ramasse[4], Detlev Grützmacher[1], and Beata Kardynał[1] — [1]PGI 9, Forschungszentrum Jülich, Jülich, Germany — [2]II. Physikalisches Institut, Georg-August-University Göttingen, Göttingen, Germany — [3]Department of Physics, Univsity of Limerick, Limerick, Ireland — [4]SuperSTEM Laboratory, Daresbury, UK

Monolayer transition metal dichalcogenides (TMDs) have gained interest as material for optoelectronics. In order to realise the technological potential of the TMDs semiconductors, it is desirable to be able to form heterostructures and introduce dopants in the monolayers. In this study, we examine the possibility to do so using ion implantation. We show that chalcogen atoms of the monolayer MoS2 can be substituted using very low energy ion beams (<50 eV) as verified using Raman spectroscopy and scanning transmission electron microscopy. Implantation levels of a few percent are realised with no structural damage visible in Raman spectra. Significant changes of the photoluminescence compared with pristine MoS2 monolayers are observed at cryogenic temperature. The technique under development is to be applied for forming lateral heterostructures of 2D TMDs.

TT 9.9 Mon 17:45 POT 81

synthesis of bismuth/reduced graphene oxide composites and their electrochemical properties for Na-ion batteries — •Benrong Hai[1,2], Yang Xu[1], Min Zhou[1], Liying Liang[1], and Yong Lei[1] — [1]TU-ilmenau, Ilmenau, Germany — [2]Northeastern University, Shenyang, P. R. China

Recently, Na-ion batteries have been considered as a desirable alternative to Li-ion batteries, because of the greater abundance and lower cost of sodium-containing precursors. Even though Na-ion batteries have attracted great attention, more research is needed to enhance their performance. Reduced graphene oxide sheets have extraordinary electronic transport properties, large surface area and mechanical flexibility. Therefore, reduced graphene oxide sheets have been considered as a matrix material to improve electrochemical performance of metal nanoparticles. Here, we demonstrate a facile strategy to prepare bismuth/reduced graphene oxide composites. Such composites exhibit high specific capacity and enhanced cycling performance as anode. Compared to pure bismuth nanoparticles, the enhancement of sodium storage could be attributed to the introduction of reduced graphene oxide sheets that not only buffer the large volume changes during the reaction of sodium and bismuth, but also provide a highly conductive network for rapid electron transport in electrochemical reaction.

TT 9.10 Mon 18:00 POT 81

Optical properties of boron vacancies and boron vacancy complexes in hexagonal boron nitride — •Mažena Mackoit and Audrius Alkauskas — Center for Physical Sciences and Technology, Vilnius, Lithuania

In this work we perform density functional theory calculations of boron vacancies and boron vacancy complexes with oxygen in hexagonal boron nitride. It is shown that interaction with oxygen significantly lowers the formation energy of boron vacancies. Therefore, when oxygen is present, complexes are more likely to occur that bare vacancies. We find that electronic defect states can be of both σ and π type. This gives rise to various possible configurations of ground and excited states. In particular, it is suggested that intra-defect luminescence can be polarized both in- and out-of-plane. We also provide estimates of intra-defect excitation energies and associated Franck-Condon shifts, making the connection with recent experimental observations of single photon emitters in this material.

TT 10: Spintronics II (joint session DS, HL, MA, TT, organized by HL)

Time: Monday 14:45–17:00 Location: POT 151

TT 10.1 Mon 14:45 POT 151

Observation of suppressed electron giant-Zeeman splitting in a (Cd,Mn)Te/(Cd,Mg)Te quantum well — •Janina J. Schindler[1], Jörg Debus[1], Victor F. Sapega[2], Dmitri R. Yakovlev[1,2], Grzegorz Karczewski[3], Tomasz Wojtowicz[3], and Manfred Bayer[1,2] — [1]Experimental Physics 2, TU Dortmund University, Dortmund, Germany — [2]Ioffe Institute, Russian Academy of Sciences, St. Petersburg, Russia — [3]Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

We have studied the electron spin properties in a (Cd,Mn)Te/(Cd,Mg)Te quantum well modulation-doped with a high-mobile, highly concentrated two-dimensional electron gas by means of resonant spin-flip Raman scattering (SFRS). Resonant SFRS is a spin manipulating optical tool that also provides insight in spin interaction processes and spin-level structures. Two electron-SFRS signals with sharp resonance profiles at about 1.594eV and 1.599eV are observed, both showing no exciton-exchange energy offset at 0 T. The Mn-ion interactions with carriers in diluted magnetic semiconductors (DMS) lead typically to the giant Zeeman splitting of the electron and hole spin states with effective g-factors in the range of 10 to 80. However, the electron-SFRS signals demonstrate an effective g-factor of -1.7, which is characteristic for non-magnetic II-VI quantum wells. The optical selection rules derived from the circular polarization features let us assume that the SFRS processes involve a negative trion with componensated electron spins or a highly localized exciton bound to an impurity in the (Cd,Mn)Te quantum well.

TT 10.2 Mon 15:00 POT 151

Optical control of a strongly coupled spin-spin system in ZnO — Jan Heye Buss[1], Jörg Rudolph[1], Thomas A. Wassner[2], Martin Eickhoff[3], and •Daniel Hägele[1] — [1]Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum, D-44780 Bochum — [2]Walter Schottky Institut, Technische Universität München, D-85748 Garching — [3]Justus-Liebig-Universität Gießen, I. Physikalisches Institut, D-35392 Gießen

The electron spin of the indium donor in ZnO couples strongly to the 9/2 nuclear spin of indium providing a non-trivial quantum system that can be optically manipulated and read out. Time-resolved Kerr-rotation measurements show directly a complex beating behavior of the electron spin under the application of an external magnetic field. The beat-structure provides a fingerprint of the 10 nuclear spin levels. We find evidence for an efficient optical pumping of the nuclear spin state via the optically pumped donor electron. A modulated pump pulse polarization reduces the nuclear spin polarization starting at frequencies above 100 kHz reaching zero polarization at 8 MHz. A full quantum mechanical modeling of the system including spin relaxation, optical pumping, and electron hopping exhibits excellent agreement with experiment [1]. Prospects for creating non-classical nuclear spin states will be discussed.

[1] J. H. Buß, J. Rudolph, T. A. Wassner, M. Eickhoff, and D. Hägele, Phys. Rev. B 93, 155204 (2016)

TT 10.3 Mon 15:15 POT 151

Design of polarization degenerate photonic nanocavities for cavity-enhanced optical spin-pumping — •Tobias M. Petzak[1], Sebastian Hammer[1,2], and Hubert J. Krenner[1,2] — [1]Lehrstuhl für Experimentalphysik 1, Institut für Physik, Universität Augsburg, Universitätsstr. 1 86159 Augsburg, Germany — [2]Nanosystem Initiative Munich (NIM), Schellingstraße 4, 80339 München, Germany

Defect cavities in photonic crystal membranes exhibit high quality factors and enable the efficient confinement of light within small volumes. Therefore, these nanoscale optical cavities can enhance the light-matter interaction between cavity photons and optical excitations of embedded semiconductor nanosystems.

Here, we propose and demonstrate by finite-difference-time-domain (FDTD) simulations, that a crossed-beam cavity design [1] allows to obtain polarization-degenerate photonic modes. This is achieved by varying the geometry of the two perpendicular cavities. The resulting tunable superposition of two linear polarized modes permits for the formation of a single and completely unpolarized mode. Such polarization properties are highly desirable for optically addressing spin- and valley degrees of freedom e.g. in monolayer transition metal dichalcogenides [2]. We show that our design can be implemented on thermally grown SiO_2 for which our FDTD simulations predict quality factors exceeding 300 for cavities resonant with the exciton transition of WS_2.

References:
[1] K. Riviore et al., *Appl. Phys. Lett.* **99**, 013114 (2011)
[2] K. F. Mak et al., *Nature Nanotechnology* **4**, 494-498 (2012)

TT 10.4 Mon 15:30 POT 151

Anisotropy of the spin diffusion in GaAs-based two-dimensional electron gases — •Markus Schwemmer[1], Andreas Hanninger[1], Dieter Schuh[1], Werner Wegscheider[2], Tobias Korn[1], and Christian Schüller[1] — [1]Institute of Experimental and Applied Physics, Faculty of Physics, University of Regensburg, Germany — [2]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 two-dimensional electron system (2DES) based on a modulation-doped AlGaAs/GaAs quantum well. The electron spin dynamics, and thus the electron spin diffusion, is determined by the interplay between Dresselhaus and Rashba fields. The geometry of the Dresselhaus field, which arises due to the bulk inversion asymmetry, is mostly determined by the growth direction of the quantum well. The Rashba field instead is caused by a structure inversion asymmetry, which can be controlled, e.g. by the modulation doping. For the specific case of a symmetrically modulation-doped, (110)-grown GaAs quantum well, optically injected electron spins align parallel or antiparallel to the spin-orbit field. Therefore, D'yakonov-Perel spin dephasing is suppressed and a long spin coherence time can be attained. For such a system one would expect naively isotropic electron spin diffusion in the quantum well plane. Nevertheless a strongly direction-dependent behaviour of the electron spin diffusion is observed.

Coffee Break

TT 10.5 Mon 16:15 POT 151

Higher-order quantum theory of spin noise spectroscopy — •Daniel Hägele — Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum, D-44780 Bochum

Spin noise spectroscopy has recently evolved into a versatile tool for studying spin dynamics in atoms and solids with minimal perturbation of the quantum system. A fully quantum mechanical theory of the detector output $z(t)$ is highly desirable for calculating higher order spectra of complex spin systems taking into account measurement back-action and relaxation. Treating spin noise spectroscopy within a stochastic master equation approach we find $z(t)$ in all orders of the measurement strength β [1]. This continuous quantum noise formula (CQNF) depends non-linearly on the equilibrium density matrix ρ_0 and contains as further ingredients the system propagator $G(t)$, the measurement operator σ_z, and multiple convolutions with white Gaussian noise $\Gamma(t)$. The CQNF allows for a systematic derivation of the spin noise spectrum $S_{\mathrm{q}}(\omega) = \frac{1}{2}\left(\mathrm{Tr}\left[(\sigma_z - \mathrm{Tr}(\sigma_z\rho_0))G(\omega)(\sigma_z\rho_0 + \rho_0\sigma_z)\right] + \mathrm{c.c.}\right)$ and higher order spectra such as the bispectum and trispectrum. The CQNF may also be applied to transport theory and measurement theory in general.

[1] D. Hägele, https://arxiv.org/abs/1611.02077

TT 10.6 Mon 16:30 POT 151

Off-diagonal g-tensor components in [113]-grown two-dimensional hole systems — •Christian Gradl[1], Michael Kempf[1], Johannes Holler[1], Roland Winkler[2], Dieter Schuh[1], Dominique Bougeard[1], Christian Schüller[1], and Tobias Korn[1] — [1]Universität Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, Northern Illinois University, DeKalb, Illinois 60115, USA

Due to its p-like character, the valence band in GaAs-based heterostructures offers rich and complex spin-dependent phenomena. Especially for some low-symmetry growth directions, off-diagonal components of the hole g-tensor are theoretically predicted. Therefore, we perform time-resolved Kerr rotation measurements on an undoped [113]-grown double quantum well (QW) structure to resolve the spin dynamics of hole ensembles at low temperatures. By varying the di-

rection of the applied magnetic field, we observe a non-diagonal hole g-tensor and quantify the individual tensor components, which are in very good agreement with our theoretical calculations.

TT 10.7 Mon 16:45 POT 151

An origin of large spin accumulation voltage in non-degenerate Si MOSFET at room temperature — •Masashi Shiraishi[1], Yuichiro Ando[1], Takayuki Tahara[1], and Hayato Koike[2] — [1]Kyoto University, Japan — [2]TDK Corporation, Japan

Si spintronics has been attracting much attention in a decade, and recent success of room temperature operation of Si spin MOSFET [1] can accelerate its progress. In this presentation, a large spin accumulation voltage of more than 1.5 mV at 1 mA measured in non-degenerate Si-based lateral spin valves (LSVs) at room temperature is introduced [2]. The notable is that this is the largest spin accumulation voltage measured in semiconductor-based LSVs in our best knowledge. The modified spin drift-diffusion model, which successfully accounts for the spin drift effect, explains the large spin accumulation voltage and significant bias-current-polarity dependence. The model also shows that the spin drift effect enhances the spin-dependent magnetoresistance in the electric two-terminal scheme. This finding provides a useful guiding principle for spin metal-oxide-semiconductor field-effect transistor operations. The detail of experiments and theoretical considerations will be introduced in the presentation. Reference:[1] T. Tahara, M. Shiraishi et al., APEX8, 113004 (2015). [2] T. Tahara, M. Shiraishi et al., Phys. Rev. B93, 214406 (2016).

TT 11: SYCE: Novel Functionality and Topology-Driven Phenomena in Ferroics and Correlated Electron Systems (joint symposium DF, DS, KR, MA, MI, TT, organized by DS)

Time: Monday 15:00–18:00 Location: HSZ 02

Invited Talk TT 11.1 Mon 15:00 HSZ 02

Ferroelectric domain walls: from conductors to insulators and back again — •Petro Maksymovych — Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, USA

The root cause of uncertainty around conducting ferroelectric domain walls (DWs) is the contact problem, which may be intrinsic to the polarization topology and may not be resolved by doping ferroelectric films. We revealed how contact effects are responsible for apparent DW conductance in ultrathin BiFeO3, wherein the DW electrostatically gates the interface, but is not itself a conductor. At the same time, we explored AC conductance of DWs to eliminate contact effects. DWs in both BiFeO3 and Pb(Zr0.2Ti0.8)O3 revealed robust conductivity at 3 GHz with remarkably large values of 2-6 S/m. Using the Ginzburg-Landau-Devonshire model for ferroelectric semiconductor, the effect is traced to local charge of nominally straight DWs due to defect-induced roughening and/or an intrinsic flexoelectric effect. Microwave regime opens new opportunities for device integration and carrier-density and dielectric effects at DWs.

Support provided by U.S. Department of Energy, BES, Materials Science and Technology Division. Microscopy experiments performed at the Center for Nanophase Materials Sciences, a DOE Office of Science User Facility.

[1] R. K. Vasudevan, et al., and P. Maksymovych, submitted (2016) [2] A. Tselev, P. Yu, Y. Cao, L. R. Dedon, L. W. Martin, S. V. Kalinin, and P. Maksymovych, Nat. Comms., 7 (2016) 11630.

Invited Talk TT 11.2 Mon 15:30 HSZ 02

Zoology of skyrmions and the role of magnetic anisotropy in the stability of skyrmions — •Istvan Kezsmarki[1], Sandor Bordacs[1], Jonathan White[2], Vladimir Tsurkan[3], Alois Loidl[3], Peter Milde[4], Hiroyuki Nakamura[5], and Andrey Leonov[6] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]Paul Scherrer Institute, Villingen, Switzerland — [3]University of Augsburg, Augsburg, Germany — [4]Technical University of Dresden, Dresden, Germany — [5]University of Kyoto, Kyoto, Japan — [6]University of Hiroshima, Hiroshima, Japan

Skyrmions are nanometric magnetic objects with high stability owing to their topological structures. The internal spin pattern of skyrmions depends on the crystal symmetry of the host materials. While we know many chiral crystals hosting Bloch-type skyrmions, Néel-type skyrmions have only recently observed in polar compounds. On experimental basis, I am going to compare the main characteristics of the two types of skyrmions and discuss the effect of magnetic anisotropy on the thermal stability range of the corresponding Bloch- and Néel-type skyrmion lattices.

Invited Talk TT 11.3 Mon 16:00 HSZ 02

Magnetic imaging of topological phenomena in ferroic materials — •Weida Wu — Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, 08854 USA

Topology is a pervasive concept in condensed matter physics. Topological phenomena such as vortices, Skyrmions and chiral edge states are mesoscopic textures that are crucial for the physical properties and functionalities. Thus, it is imperative to directly visualize these mesoscopic phenomena. In this talk, I will present our recent discovery of alternating uncompensated magnetic moments at Z6 vortex domain walls in hexagonal manganites, which demonstrates the coupling between ferroelectric and antiferromagnetic orders. Furthermore, magnetoelectric response of the vortex domains were directly visualized by Magnetoelectric Force Microscopy (MeFM), a combination of MFM with in-situ modulating high electric fields. Our MeFM results reveal a giant enhancement of magnetoelectric response of a lattice mediated magnetoelectric effect near a spin-reorientation critical point.

This work is supported by US DOE under grant DE-SC0008147.

30 min. break

Invited Talk TT 11.4 Mon 17:00 HSZ 02

Topological skyrmion textures in chiral magnets — •Markus Garst — Institut für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01062 Dresden, Germany

A magnetization that spatially varies within a plane can be characterized by a topological skyrmion number specifying how often the magnetization vector covers the unit sphere. Magnetic skyrmion textures with such a non-trivial winding number are endowed with additional functionality as they efficiently couple to magnon- and itinerant spin currents allowing for novel spintronic applications. Such textures arise, in particular, in chiral magnets where the Dzyaloshinskii-Moriya interaction favours a spatially modulated magnetization. This stabilizes magnetic solitons that carry an integer skyrmion charge as well as regular arrangements thereof, i.e., skyrmion crystals. We demonstrate that defects of helimagnetic order can carry half-integer skyrmion numbers. In analogy to cholesteric liquid crystals, such defects can be interpreted as disclinations and dislocations that are instrumental for the magnetic relaxation process in these systems. We also show that an array of such defects might arise in topological domain walls of helimagnetic order permitting an efficient manipulation by spin currents.

Invited Talk TT 11.5 Mon 17:30 HSZ 02

Learning through ferroelectric domain dynamics in solidstate synapses — Sören Boyn[1], Gwendal Lecerf[2], Stéphane Fusil[1], Sylvain Saïghi[2], Agnès Barthélémy[1], Julie Grollier[1], Vincent Garcia[1], and •Manuel Bibes[1] — [1]Unité Mixte de Physique CNRS/Thales, Palaiseau FRANCE — [2]IMS Laboratory, U. Bordeaux FRANCE

In the brain, learning is achieved through the ability of synapses to reconfigure the strength by which they connect two neurons. Artificial hardware with performances emulating those of biological systems require electronic nanosynapses endowed with such plasticity. Promising solid-state synapses are memristors, simple two-terminal nanodevices that can be finely tuned by voltage pulses. Their conductance evolves according to a learning rule called spike-timing-dependent plasticity, conjectured to underlie unsupervised learning in our brains. We will report on purely electronic ferroelectric synapses and show that spike timing-dependent plasticity can be harnessed and tuned from intrinsically inhomogeneous ferroelectric polarisation switching. Through combined scanning probe imaging and electrical transport experiments, we demonstrate that conductance variations in such BiFeO3-based ferroelectric memristors can be accurately controlled and modelled by the nucleation-dominated electric-feld switching of domains

with different polarisations. Our results show that ferroelectric nanosynapses are able to learn in a reliable and predictable way, opening the way towards unsupervised learning in spiking neural networks.

TT 12: Correlated Electrons: Frustrated Magnets - General 1

Time: Monday 15:00–18:15 Location: HSZ 03

TT 12.1 Mon 15:00 HSZ 03

Excitations of the Shastry-Sutherland model in the plaquette phase — •Carolin Boos[1], Frédéric Mila[2], and Kai Schmidt[1] — [1]FAU Erlangen-Nürnberg, Deutschland — [2]EPF Lausanne, Schweiz

The quantum magnet $SrCu_2(BO_3)_2$ is well described by the two-dimensional Shastry-Sutherland model, that is a frustrated spin-1/2 system on a square lattice with some next-nearest-neighbor interactions. Under pressure a quantum phase transition is observed in $SrCu_2(BO_3)_2$, which is suggested to correspond to the plaquette phase of the Shastry-Sutherland model. In this work we study the excitation spectrum of the plaquette phase to clarify the presence of this phase in $SrCu_2(BO_3)_2$.
To this end we consider a high-order linked-cluster expansion using perturbative continous transformations about the isolated plaquette limit. We calculate the dispersion and compare it with inelastic neutron scattering results of $SrCu_2(BO_3)_2$ under a pressure of 21.5 kbar from [1].

[1] M.E. Zayed *et al.*, ArXiv:1603.02039v1, 2016.

TT 12.2 Mon 15:15 HSZ 03

Anisotropic kagome lattice as the origin of canted antiferromagnetism in barlowite — •Alexander A. Tsirlin[1], Ronald Zinke[2], Ioannis Rousochatzakis[3], Helge Rosner[4], and Johannes Richter[2] — [1]EP VI, EKM, University of Augsburg, Germany — [2]Institute of Theoretical Physics, University of Magdeburg, Germany — [3]School of Physics, University of Minnesota, Minneapolis, US — [4]MPI for Chemical Physics of Solids, Dresden, Germany

Barlowite is a recent addition to the family of spin-$\frac{1}{2}$ kagome minerals that, despite its reported three-fold symmetry of the crystal structure, reveals long-range magnetic order below 15 K with a weak remnant magnetization. Using density-functional band-structure calculations along with the effective theory and coupled-cluster method for spin Hamiltonians, we propose that the disordered arrangement of the interlayer Cu site gives rise to a tangible deformation of the kagome layers. Their local configurations can be represented by a combination of weakly coupled linear trimers and spatially anisotropic kagome lattice. While the former give rise to simple antiferromagnetic order, the latter supports canted antiferromagnetic order driven by quantum fluctuations and reinforced by Dzyaloshinsky-Moriya anisotropy. This mechanism stabilizes canted antiferromagnetic order with a relatively low net moment lying in the kagome plane, which is only possible when geometrical distortion of the kagome lattice is taken into account.

TT 12.3 Mon 15:30 HSZ 03

Magnetic resonance as a local probe for $S = \frac{1}{2}$ Kagomé magnetism in Barlowite $Cu_4(OH)_6FBr$ — •Ranjith Kumar Kizhake Malayil[1], Christian Klein[2], Cornelius Krellner[2], and Michael Baenitz[1] — [1]MPI for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Institute of Physics, Goethe-University Frankfurt, 60438 Frankfurt am Main, Germany

$S = \frac{1}{2}$-quantum magnets with Kagomé 2D layer building blocks could serve as model systems for 2D magnetic frustration and may host the quantum spin liquid state (QSL). So far Herbertsmithite (HS) $ZnCu_3(OH)_6Cl_2$ is the leading candidate for this research, but here structural disorder has some influence on the QSL state. Barlowite, $Cu_4(OH)_6FBr$ is a relative to HS and is predicted to host an undistorted Kagomé lattice [1].

Here, we present ^{1}H, ^{19}F, and ^{79,81}Br NMR measurements together with a Br-NQR study on polycrystalline samples to probe the magnetism, the magneto elastic coupling and the local disorder. From spin-lattice relaxation results strong evidence for magnetic order at 15 K is given. Furthermore, a large field dependence of the hyperfine fields is observed. This is discussed to originate from a weak out of plane magnetic exchange interaction.

[1] Han et al., Phys. Rev. Lett. **113**, 227203 (2014).

TT 12.4 Mon 15:45 HSZ 03

Electronic Excitations and Lattice Vibrations on the Kagome Lattice: Herbertsmithite and Related Compounds — •Andrej Pustogow[1], Mathias Bories[1], Ievgen Voloshenko[1], Pascal Puphal[2], Cornelius Krellner[2], Ying Li[2], Roser Valenti[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Physikalisches Institut, Universität Frankfurt

We present a broadband optical and theoretical study of the electrodynamic response of the quantum spin liquid candidate Herbertsmithite and related Kagome lattice compounds. At low frequencies the spectrum of these frustrated Mott insulators is dominated by phonons. We assign the lattice vibrations within and perpendicular to the Kagome layer on the basis of theoretical calculations. In the visible and ultraviolet ranges we identify interband transitions and relate them to recent band structure calculations. Finally, we tackle the open question about the theoretically predicted contribution of spinon excitations to the low-frequency optical conductivity.

TT 12.5 Mon 16:00 HSZ 03

New kagome systems $YCu_3(OH)_6Cl_3$ and $Ga_xCu_{4-x}(OH)_6Cl_2$ — •Pascal Puphal[1], Michael Bolte[1], Denis Sheptyakov[2], Andrej Pustogow[3], Martin Dressel[3], Michael Baenitz[4], and Cornelius Krellner[1] — [1]Goethe-University Frankfurt am Main — [2]Laboratory for Neutron Scattering and Imaging, PSI, Villigen — [3]1. PI, Stuttgart University — [4]MPI-CPfS, Dresden

Herbertsmithite $ZnCu_3(OH)_6Cl_2$ is a highly frustrated kagomé system, which has an antiferromagnetic superexchange interaction of J = 17 meV, but no long-range order has been observed down to T = 50 mK. We have successfully prepared $Ga_xCu_{4-x}(OH)_6Cl_2$, with a three valent ion instead of Zn^{2+}, which should lead to a Dirac metal as proposed by I. I. Mazin et. al. [1]. We synthesized powder samples of this compound with different substitution amounts of $x < 1$. Similar to Zn the increasing Ga amount slowly suppresses the ordering at 6.5 K, but the compound stays insulating which is also reflected in its green colour. We show magnetometry, specific heat as well as optical and local probing data like NMR. The second part of the contribution is about $YCu_3(OH)_6Cl_3$ which shows a new kapellasite like structure. Using hydrothermal growth we synthesized single crystals of up to 2 x 2 x 0.5 mm. The structure is a slightly distorted kagome layer with two copper positions giving a new two-dimensional frustrated arrangement. The susceptibility as well as specific heat show a weak antiferromagnetic ordering at 2.2 K while the system has a Weiss temperature of -104 K resulting in a frustration coefficient of 50.

[1] I. I. Mazin et al., Nature Communications 5, 4261 (2014)

TT 12.6 Mon 16:15 HSZ 03

Spin Frustration in an Organic Radical Ion Salt Based on a Kagome-Coupled Chain Structure — •Lars Postulka[1], Stephen M. Winter[1], Bernd Wolf[1], Adam G. Mihailov[2], Aaron Mailman[2], Adbeljalil Assoud[2], Craig M. Robertson[3], Richard T. Oakley[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe Universität, SFB/TR49, Frankfurt, DE — [2]Dep. of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada — [3]Dep. of Chemistry, University of Liverpool, Liverpool L69 7ZD, United Kingdom

Frustrated quantum spin systems have attracted enormous interest in experimental and theoretical studies as these systems are expected to host spin liquid states. A model system for such frustrated quantum magnets is the kagome lattice with S=1/2 moments at the lattice vertices. Here we present a purely organic variant built out of quinoidal bisdithiazole $[BT]^+$ radicals and $[GaBr_4]^-$.The packing pattern of the radical cations provides a rare example of an organic kagome basket structure. Magnetic measurements over a wide temperature range 30 mK $< T <$ 300 K suggest strongly frustrated AFM interactions of the scale of $J/k_B \approx 30$ K, but reveal no anomalies that would be associated with magnetic order. The high-temperature part of the susceptibility can be described in a coupled-chain model. By combining results from high-temperature series expansion and density functional theory we

could resolve that these chains are coupled in a distorted kagome lattice[1].

[1] L. Postulka et al., J. Am. Chem. Soc. 138, 10738 (2016)

15 min. break.

TT 12.7 Mon 16:45 HSZ 03

Anisotropy governed competition of magnetic phases in the honeycomb quantum magnet $Na_3Ni_2SbO_6$ — •Johannes Werner[1], Waldemar Hergett[1], Mario Gertig[1], Jaena Park[1], Changhyun Koo[1], and Rüdiger Klingeler[1,2] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Centre for Advanced Materials, Heidelberg University, Heidelberg, Germany

Thermodynamic properties as well as low-energy magnon excitations of the layered $S = 1$ honeycomb-lattice system $Na_3Ni_2SbO_6$ have been studied by high-resolution dilatometry, high-field magnetometry, and antiferromagnetic resonance (AFMR) studies in magnetic fields up to 18 T. At $T_N = 16.5$ K, there is a tricritical point separating two antiferromagnetic phases AF1 and AF2 from the paramagnetic regime. In the AF1 phase below $B_{C1} \approx 9.5$ T (at 4.2 K), the AFMR modes suggest a two-sublattice spin configuration which is consistent with stripe-like order. Observed zero field splitting $\Delta_{ZFS} = 360$ GHz of the AFMR modes indicates an uniaxial anisotropy field $B_A = 1.7$ T. We conclude the crucial role of the axial anisotropy favoring the AF1 spin structure over the AF2 one. While magnetostriction data disprove a simple spin-flop scenario at B_{C1}, the nature of a second transition at $B_{C2} \approx 13$ T remains unclear. Both the sign of the magnetostriction dL/dB and Grüneisen scaling suggest that short-range antiferromagnetic correlations present at least up to $\sim 5 \cdot T_N$ are of AF2-type, i.e. the intermediate field phase.

TT 12.8 Mon 17:00 HSZ 03

Quantum anomalous Hall state in ferromagnetic $SrRuO_3$ (111) bilayers — Liang Si[1], •Oleg Janson[1], Gang Li[1], Zhicheng Zhong[2], Zhaoliang Liao[3], Gertjan Koster[3], and Karsten Held[1] — [1]Institut für Festkörperphysik, TU Wien, Vienna, Austria — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

We study electronic, magnetic and topological properties of the honeycomb lattice formed by $SrRuO_3$ (111) bilayers by means of density functional theory, dynamical mean field theory (DMFT) and model simulations. DMFT yields a half-metallic ferromagnetic state below 500 K with an ordered magnetic moment of $2\,\mu_B$. In the minority channel, the spin-orbit coupling opens a gap at the linear band crossing corresponding to 4/3 filling of the $4d$ t_{2g} shell. Using model calculations, we demonstrate that the respective state is a quantum anomalous Hall state and discuss possible routes towards an experimental realization of this topological states.

OJ acknowledges the support by the Lise Meitner Programme of Austrian Science Fund (FWF), project M2050.

Invited Talk TT 12.9 Mon 17:15 HSZ 03

U(1) Quantum Spin Liquid Ground State in the Triangular Antiferromagnet $YbMgGaO_4$ — •Yuesheng Li — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg

Quantum spin liquids are novel phases of matter, where spins are entangled up to long-distances and times without symmetry breaking even at 0 K due to the strong quantum fluctuations. And the candidate materials were actively sought after. However, most of the existing candidates suffer from magnetic defect, lattice distortion, antisymmetric exchange (Dzyaloshinskii-Moriya interactions) and (or) interlayer magnetic coupling. Recently, a new structurally perfect triangular antiferromagnet $YbMgGaO_4$ was reported by our group [1,2]. The aforementioned structural shortcomings are avoided [1]. (1) No spin symmetry breaking is detected down to 0.048 K [1,3], and the spin entropy is precisely measured to be almost zero at 0.06 K [1]. (2) The measured magnetic heat capacity behaves as $C_m \sim T^{2/3}$ down to 0.06 K under 0 T [1]. (3) The muon spin relaxation rates exhibit temperature-independent plateaus below 0.4 K [3]. (1)-(3) suggest $YbMgGaO_4$ may be the first experimental realization of the U(1) quantum spin liquid ground state.

[1] Yuesheng Li et al., Sci. Rep. 5, 16419 (2015)
[2] Yuesheng Li et al., Phys. Rev. Lett. 115, 167203 (2015)
[3] Yuesheng Li et al., Phys. Rev. Lett. 117, 097201 (2016)

TT 12.10 Mon 17:45 HSZ 03

Tuning the Effective Correlations in a Mott Insulator and Quantum Spin Lquid Compound — Miriam Sanz Alonso[1], Andrej Pustogow[1], Yohei Saito[2], Atsushi Kawamoto[2], and •Martin Dressel[1] — [1]1. Phys. Inst. Univ. Stuttgart, Germany — [2]Div. of Phys. Hokkaido Univ., Sapporo, Japan

The fictitious state of a quantum spin liquid was first realized in the dimerized Mott system κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ about a decade ago. Here we tune the effective correlations U/W by a gradual increase of the bandwidth W in the substitutional series κ-(BEDT-TTF$_{1-x}$BEDT-STF$_x$)$_2$Cu$_2$(CN)$_3$ with $0 \leq x \leq 1$, where on one side of the molecule sulfur has been replaced by the larger selenium atoms. Comprehensive optical and transport investigations down to low temperatures evidence a metal-insulator transition as x exceeds 20% with no indications that disorder plays a crucial role. We analyze the dynamics of the correlated charge carriers and the shift of spectral weight; the results allow us to generate a unified phase diagram of this Mott system, that remains a spin liquid as it does not exhibit magnetic order down to lowest temperatures.

TT 12.11 Mon 18:00 HSZ 03

Quantum Monte-Carlo study of hardcore bosons on a kagome lattice — •Xue-Feng Zhang[1], Yin-Chen He[2], Sebastian Eggert[3], Roderich Moessner[1], and Frank Pollmann[1] — [1]Max-Planck- Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Department of Physics, Harvard University, Cambridge, MA 02138, USA — [3]Physics Department and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

We study an extended Hubbard model of hardcore bosons on the kagome lattice. In the limit of strong nearest-neighbor interactions at one-third filling, the interplay between frustration and quantum fluctuation is know to form a valence bond solid. When decreasing the interaction strength, the system has a transition to a superfluid phase. The precise nature of this phase transition is still under debate. Two possibilities are that it could be a weakly first order or an unconventional continuous phase transition. We revisit this problem using large scale quantum Monte Carlo simulation with parallel tempering. We find a first order phase transition away from the tip of the one third filling lobe, while it appears to be continuous at exactly one third filling. A careful finite size scaling analysis reveals an unconventional scaling behavior hinting at deconfined quantum criticality.

TT 13: Superconductivity: Fe-based Superconductors - 122

Time: Monday 15:00–18:15 Location: HSZ 103

TT 13.1 Mon 15:00 HSZ 103

Fermi surface and effective masses in photoemission response of the K doped $BaFe_2As_2$ superconductor — Gerald Derondeau[1], Federico Bisti[2], Jürgen Braun[1], Hubert Ebert[1], Vladimir Strocov[2], and •Jan Minar[1,3] — [1]LMU München, Germany — [2]Swiss Light Source, PSI, Villigen, Switzerland — [3]University of West Bohemia, Pilsen, Czech Republic

The angle-resolved photoemission spectra of the K doped superconductor $BaFe_2As_2$ have been investigated both experimentally and theoretically. Our results explain the previously obscured origins of all salient features of the ARPES response of this paradigm pnictide compound and reveal the origin of the Lifshitz transition. Comparison of calculated ARPES spectra with the underlying DMFT band structure shows an important impact of final state effects, which results for three-dimensional states in a deviation of the ARPES spectra from the underlying spectral function. In particular, the apparent effective mass enhancement seen in the ARPES response is not an entirely intrinsic property of the quasiparticle valence bands but has a significant extrinsic contribution from the photoemission process and thus differ from its true value. Because this effect is more pronounced for low photoexcitation energies, soft-X-ray ARPES delivers more accurate values of the mass enhancement due to a sharp definition of the 3D electron momentum.

TT 13.2 Mon 15:15 HSZ 103

Nematic susceptibility of hole-doped $Ba_{1-x}Na_xFe_2As_2$ iron pnicdies studied by shear-modules measurements — •Liran Wang[1], Frédéric Hardy[1], Mingquan He[1], Liping Xu[1,2], Peter Schweiss[1], Thomas Wolf[1], and Christoph Meingast[1] — [1]Institute für Festkörperphysik,Karlsruher Institut für Technologie (KIT), 76344 Karlsruhe, Germany — [2]Key Laboratory of Polar Materials and Devices, Department of Electronic Engineering, East China Normal University, Shanghai 200241, China

In order to study the complex electronic phase diagram of hole-doped doped $Ba_{1-x}Na_xFe_2As_2$[1] iron based superconductor, we investigate the nematic susceptibility extracted from shear modulus data obtained using a three-point-bending method[2,3] in a capacitance dilatometer. Other complimentary measurements, including thermal expansion[4], specific heat, as well as transport, have also been performed on this system. We find that the nematic susceptibility of doped $Ba_{1-x}Na_xFe_2As_2$ does not follow a Curie-Weiss temperature dependence over the entire doping region, which is in contrary to the electron-doped $Ba(Fe_{1-x}Co_x)_2As_2$ yet similar to its analogue $Ba_{1-x}K_xFe_2As_2$[2]. In particular, we find a large increase of the nematic susceptibility upon entering the $C4$ magnetic phase.

[1] L. Wang et al., Phys. Rev. B 93, 014514 (2016)
[2] A. Böhmer et al., Phys. Rev. Lett. 112, 047001 (2014)
[3] A. Böhmer et al., Comptes Rendus Physique 17, 1-2, 90-112 (2016)
[4] C. Meingast et al, Phys. Rev. B 41, 11299 (1990)

TT 13.3 Mon 15:30 HSZ 103

Search for broken time reversal symmetry of the superconducting order parameter in $Ba_{1-x}K_xFe_2As_2$ — •Vadim Grinenko[1], Philipp Materne[1], Rajib Sarkar[1], Sirko Kamusella[1], Hubertus Luetkens[2], Kunihiro Kihou[3], Chul-Ho Lee[3], Shavkat Akhmadaliev[4], Dmitriy Efremov[5], Stefan-Ludwig Drechsler[5], and Hans-Henning Klauss[1] — [1]Institute for Solid State Physics, TU Dresden, D-01069, Germany — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute (PSI), CH-5232 Villigen, Switzerland — [3]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8560 Japan — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [5]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

Multi-band iron pnictides superconductors provide a unique possibility to study the effect of competing interactions on the superconducting (SC) order parameter symmetry. In $Ba_{1-x}K_xFe_2As_2$ a change of the SC order parameter symmetry at high K doping level x was predicted theoretically by S. Maiti *et al.*, Phys Rev. B **91**, 161102(R) (2015). This change occurs through an intermediate state with a complex order parameter which can lead to spontaneous currents below the SC critical temperature T_c. Here we report our muon spin rotation/relaxation (μSR) experiments on single crystalline samples of the title compound. In our experiments we observe an enhancement of the zero field muon relaxation rate below T_c for the sample with $x \approx 0.7$. This result is interpreted as an evidence for the complex SC order parameter at this doping level.

TT 13.4 Mon 15:45 HSZ 103

Effects of enhanced electron correlations on upper critical field properties in AFe_2As_2 (A = K, Rb, and Cs) superconductors — •Seunghyun Khim[1,2], Dmitry Efremov[1], Anja U. B. Wolter[1], Sabine Wurmehl[1], and Bernd Büchner[1,3] — [1]Leibniz Institute for Solid State and Materials Research, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187, Dresden — [3]Institute for Solid State Physics, TU Dresden, 01069 Dresden, Germany

Unusually large Sommerfeld coefficients (γ_0) in the stoichiometric AFe_2As_2 (A = K, Rb, and Cs) superconductors imply enhanced electron correlations which might be related to its unconventional pairing origin of superconductivity. Including experimental data from our $CsFe_2As_2$ single crystals, we summarize magnetic susceptibility and specific heat properties of the AFe_2As_2 series to clarify the impact of electron correlations on normal and superconducting states. Toward $CsFe_2As_2$, γ_0 increases to ~ 160 mJ/mol K^2 and the broad local maximum in the magnetic susceptibility systematically shifts to lower temperatures. The slope of upper critical fields near T_c is also enhanced as predicted in accordance with the growing γ_0. Taking into account these observations, the effect of the enhanced correlations on superconductivity will be discussed together with the multiband nature, orbital-selective Mottness, and suggested quantum criticality.

TT 13.5 Mon 16:00 HSZ 103

Superconductivity induced changes of phonon lifetime in $Ba(Fe_{0.94}Co_{0.06})_2As_2$ — •Maximilian Kauth[1], Frank Weber[1], Thomas Wolf[1], and Thomas Keller[2] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart

We have investigated the life time of the transversal acoustic (TA) phonon mode in the Fe-based high-temperature superconductor $Ba(Fe_{0.94}Co_{0.06})_2As_2$ along the [100] direction. We used the neutron resonant spin echo (NRSE) technique at the TRISP spectrometer at the Heinz Maier-Leibnitz Zentrum [1]. This phonon mode is the soft mode of the structural phase transition present in lower doped samples. Recent measurements showed evidence that it is sensitive to nematic fluctuations in this compound [2]. We observe a clear maximum of the TA phonon linewidth at the superconducting transition temperature $T_C \approx 24$ K. This is the first experimental evidence of changes of the phonon lifetime in Fe-based superconductors.

[1] MPI für Festkörperforschung et al., Journal of large-scale research facilities, 1, A37 (2015).
[2] F. Weber et al., arXiv:1610.00099 (2016)

TT 13.6 Mon 16:15 HSZ 103

Spin space anisotropy in Co-underdoped $BaFe_2As_2$ — •Florian Wasser[1], Chul-Ho Lee[2], Kunihiro Kihou[2], Karin Schmalzl[3], Paul Steffens[4], Navid Qureshi[1,4], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln, Germany — [2]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8568, Japan — [3]Jülich Centre of Neutron Scattering (JCNS), Forschungszentrum Jülich GmbH, Outstation at Institut Laue-Langevin, 71 avenue des Martyrs, 38000 Grenoble, France — [4]Institut Laue-Langevin, 71 avenue des Martyrs, 38000 Grenoble, France

We studied by polarised inelastic neutron scattering the spin space anisotropy in Co-underdoped $BaFe_2As_2$ in the normal as well as in the superconducting state. The spin space anisotropy in the normal state is reminiscent of the magnetic response in the pure antiferromagnetic host compound, and displays broadened spin gaps in all three directions. In particular, the longitudinal spin excitations are largely gapped by ~ 16 meV, which seems to be sufficient larger than twice the superconducting gap value and thus prohibits any interplay with superconductivity. Consequently, in the superconducting state, we observe an anisotropic spin resonance mode, which peaks at two differ-

ent energies in the two transversal spin directions respectively. The suppression of longitudinal spin fluctuations can explain the reduced superconducting transition temperature and indicates that the coexistence of antiferromagnetic order and superconductivity occurs locally.

15 min. break.

TT 13.7 Mon 16:45 HSZ 103

Nernst effect and thermal conductivity of Rh-doped $BaFe_2As_2$ — •Christoph Wuttke[1], Frank Steckel[1], Federico Caglieris[1], Seunghyun Kim[1], Sabine Wurmehl[1], Sheng Ran[2], Paul C. Canfield[2], Bernd Büchner[1,3,4], and Christian Hess[1,4] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — [3]Institut für Festkörperphysik, TU Dresden, 01069 Dresden, Germany — [4]Center for Transport and Devices, Technische Universität Dresden, 01069 Dresden, Germany

We present results for the thermal conductivity and the Nernst coefficient of electron doped $BaFe_2As_2$ with a particular focus on exploring the nematic phase. The results show a significant sensitivity of both quantities with respect to nematic fluctuations. Interestingly, the magnitude of both the Nernst effect and the thermal conductivity exhibit a non-monotonic doping dependence where the strength of fluctuations feature a local maximum in the vicinity of optimal doping. These findings reinforce the notion that nematic fluctuations play a key role for rationalizing the nature of superconductivity in iron based superconductors.

TT 13.8 Mon 17:00 HSZ 103

Selective quantum criticality in a multi-band system: $BaFe_2(As_{1-x}P_x)_2$ — •Vadim Grinenko[1,2,3], Kazumasa Iida[2], Fritz Kurth[3], Dmitriy Efremov[3], Stefan-Ludwig Drechsler[3], Ivan Cherniavskii[4], Igor Morozov[4], Jens Hänisch[5], Tobias Förster[6], Chiara Tarantini[7], Jan Jaroszynski[7], Boris Maiorov[8], Marcelo Jaime[8], Akiyasu Yamamoto[9], Ibuki Nakamura[2], Hiroyuki Fujimoto[2], Takafumi Hatano[2], Hiroshi Ikuta[2], and Ruben Hühne[3] — [1]TU Dresden, Germany — [2]Nagoya University, Japan — [3]IFW Dresden, Germany — [4]Lomonosov Moscow State University, Russian Federation — [5]Karlsruhe Institute of Technology, Germany — [6]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Germany — [7]NHMFL, Florida State University, USA — [8]MPA-CMMS, Los Alamos National Laboratory, USA — [9]Tokyo University of Agriculture and Technology, Japan

A quantum phase transition was recently reported for $BaFe_2(As_{1-x}P_x)_2$ at $x_c \sim 0.3$. For such a transition all thermodynamic and transport properties are believed to scale with a single characteristic energy, given by the quantum fluctuations. Here we reconsider this statement. We report the superconducting upper critical field H_{c2} for $BaFe_2(As_{1-x}P_x)_2$ single crystalline thin films in a wide range of P-doping by measuring the resistivity under high magnetic fields. The temperature and doping dependencies of H_{c2} signal that some parts of the Fermi surface exhibit no mass divergence at x_c in contrast to the common belief. We anticipate that the observed dual behavior could be found also in other quantum critical multi-band systems.

TT 13.9 Mon 17:15 HSZ 103

Tuning the magnetism with As - local moments in $BaFe_2As_{2-\delta}$ — •Ilka Vinçon[1,2], Rhea Kappenberger[1,2], Federico Caglieris[1], Hans-Joachim Grafe[1], Anja Wolter-Giraud[1], Christian Hess[1], Saicharan Aswartham[1], Sabine Wurmehl[1,2], and Bernd Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research Dresden IFW, Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Dresden, Germany

An important aspect of iron based superconductors is the transition from magnetically ordered to a superconducting state by doping with various elements. As a novel type of doping, partial removal of arsenic from $La(O_{1-x}F_x)FeAs_{1-\delta}$ has been shown to slightly increase the transition temperature while simultaneously creating local magnetic moments.

We present an extended analysis of arsenic deficient $BaFe_2As_{2-\delta}$ aiming to understand this unexpected behaviour. The impact of a variable arsenic deficiency on the spin density wave and local moment formation has been studied by means of magnetic susceptibility, resistivity and nuclear magnetic resonance measurements. Systematic structural changes have been determined by powder diffraction data.

TT 13.10 Mon 17:30 HSZ 103

Quantum criticality in AFe_2As_2 (A = K, Rb, Cs) superconductors probed by ^{75}As NMR spectroscopy — Z.T. Zhang[1,2], D. Dmytriieva[1,3], S. Molatta[1,3], J. Wosnitza[1,3], S. Khim[4], S. Gass[4], A.U.B. Wolter-Giraud[4], S. Wurmehl[4], H.-J. Grafe[4], and •H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden — [2]Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, China — [3]Institut für Festkörperphysik, TU Dresden, 01060 Dresden — [4]IFW Dresden, Institute for Solid State Research, 01171 Dresden

We present ^{75}As nuclear magnetic resonance measurements on single crystals of $RbFe_2As_2$ and $CsFe_2As_2$. Taking previously reported results for KFe_2As_2 into account, we find that the anisotropic electronic correlations evolve towards a magnetic instability in the AFe_2As_2 series (with A = K, Rb, Cs). Upon isovalent substitution with larger alkali ions, a drastic enhancement of the anisotropic nuclear spin-lattice relaxation rate and decreasing Knight shift reveal the formation of pronounced spin fluctuations with stripe-type modulation. Furthermore, a decreasing power-law exponent of the nuclear spin-lattice relaxation rate for in-plane applied fields evidences an emergent deviation from Fermi-liquid behavior. All these findings clearly indicate that the expansion of the lattice in the AFe_2As_2 series tunes the electronic correlations towards a quantum critical point at the transition to a yet unobserved, magnetically ordered phase.

TT 13.11 Mon 17:45 HSZ 103

Impurity effects on spin dynamics in $Ba(Fe_{1-x}Mn_x)_2As_2$ (x = 12 %) — •M. A. Surmach[1], P. Y. Portnichenko[1], J. T. Park[2], J. A. Rodriguez-Rivera[3,4], D. L. Sun[5], Y. Liu[5], C. T. Lin[5], and D. S. Inosov[1] — [1]Institut fur Festkörperphysik, TU Dresden, Germany — [2]MLZ, TU München, Garching, Germany — [3]Materials Science and Engineering, University of Maryland, USA — [4]NIST Center for Neutron Research, Gaithersburg, USA — [5]MPI fur Festkörperforschung, Stuttgart, Germany

We present new results on the structure of magnetic fluctuations in $BaFe_2As_2$ single crystals doped with Mn local moments and discuss them in relationship to the previously reported (π, π) branch of checkerboard magnetic excitations.

Mn doping introduces strong magnetic impurities, which abruptly suppress superconductivity in Fe-based compounds and evoke the second branch of diffuse short-range spin fluctuations near the (π, π) wave vector, in contrast to other iron-based superconductors, where fluctuations are limited to (π, 0) and (0, π) nesting vectors.

Our neutron spectrscopy measurements reveal the true momentum and energy dependence of the (π, π) branch of magnetic excitations along the out-of-plane (π π L) direction. We firstly showed strong three-dimensional character of these spin fluctuations, in contrast to other iron-based systems. We also report the presence of the low temperature partial spin gap along the (π π L) direction, which gradually opens below 7 meV.

TT 13.12 Mon 18:00 HSZ 103

Crystal Growth and Characterization of $BaTM_2As_2$ with TM = 3d Transition Metal — •Sebastian Selter[1], Rhea Kappenberger[1,2], Francesco Scaravaggi[1,2], Anja Wolter-Giraud[1], Sabine Wurmehl[1,2], Saicharan Aswartham[1], and Bernd Büchner[1,2] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany

To understand the role of iron as transition metal in superconductivity and magnetism in $BaTM_2As_2$, a thorough investigation with different 3d transition metals is needed. With this aim, $BaTM_2As_2$ with TM = 3d transition metal are to be investigated for trends.
Here we present a comprehensive overview on synthesis and crystal growth of $BaTM_2As_2$ with TM = 3d transition metal.
$BaCr_2As_2$, $BaMn_2As_2$, $BaCo_2As_2$, $BaNi_2As_2$ and $BaCu_2As_2$ were grown by state-of-the-art flux growth techniques. To obtain large size homogeneous crystals of $BaCr_2As_2$ and $BaCo_2As_2$, the respective growth profiles were optimized using DTA and EDS. All compounds were characterized using EDS and PXRD. A nice trend can be seen for the behavior of lattice parameters and cell volume over the exchange of TM. Additionally, first magnetic measurements were performed, showing a strong influence of TM in $BaTM_2As_2$ on the magnetic ordering.

TT 14: Superconductivity: Tunnelling, Josephson Junctions, SQUIDs 1

Time: Monday 15:00–18:15 Location: HSZ 201

TT 14.1 Mon 15:00 HSZ 201

Correlation effects in two and three-terminal superconducting nanostructures — •Vladislav Pokorny[1] and Martin Žonda[2] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University in Prague, Czech Republic

We study the effects of electron correlations on a system consisting of a single-level quantum dot attached to two superconducting and, optionally, a third metallic lead. We use the single-impurity Anderson model coupled to BCS superconducting leads to study this system and solve it using a self-consistent second-order perturbation theory method as well as the hybridization-expansion, continuous-time quantum Monte Carlo and the numerical renormalization group. We study the behavior of the Andreev subgap states, the Josephson current and the zero-pi quantum phase transition and set the limits of usability of the methods. We also show the agreement of various methods with the available experimental results.

TT 14.2 Mon 15:15 HSZ 201

Andreev spectrum of a Josephson junction with spin-split superconductors — Bogusz Bujnowski[1], •Dario Bercioux[1,2], François Konschelle[3], Jérôme Cayssol[4], and Sebastian Bergeret[1,3] — [1]Donostia International Physics Center (DIPC) - Manuel de Lardizabal 5, E-20018 San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation for Science, Maria Diaz de Haro 3, 48013 Bilbao, Spain — [3]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU E-20018 Donostia-San Sebastian, Basque Country, Spain — [4]LOMA (UMR-5798), CNRS and Université Bordeaux - F-33045 Talence, France

The Andreev bound states and charge transport in a Josephson junction between two superconductors with intrinsic exchange fields are studied. We find [3] that for a parallel configuration of the exchange fields in the superconductors the discrete spectrum consists of two pairs of spin-split states [1,2]. The Josephson current in this case is mainly carried by bound states. In contrast, for the antiparallel configuration we find that there is no spin-splitting of the bound states and that for phase differences smaller than a certain critical value there are no bound states at all. Hence the supercurrent is only carried by states in the continuous part of the spectrum. Our predictions can be tested by performing a tunneling spectroscopy of a weak link between two spin-split superconductors.

[1] P. M. Tedrow and R. Merservey, Phys. Rev. Lett., **26** 192 (1971).
[2] R. Merservey and P. M. Tedrow, Phys. Rep., **238** 173 (1994) .
[3] B. Bujnowski, *et. al*, EPL **115**, 67001 (2016).

TT 14.3 Mon 15:30 HSZ 201

Scanning tunneling spectroscopy to probe odd-triplet contributions to the long-ranged proximity effect in Al-EuS — •Simon Diesch[1], Christoph Sürgers[2], Detlef Beckmann[2], Peter Machon[1], Wolfgang Belzig[1], and Elke Scheer[1] — [1]Universität Konstanz, 78457 Konstanz, Germany — [2]Karlsruhe Institute of Technology, 76344 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 supercurrents tunneling through ferromagnetic layers, indicating Cooper pairs of equal spin, thus corresponding to a long-range triplet proximity effect [1]. Most experimental evidence for triplet superconductivity comes from observations of the thickness dependence of the Josephson current through a ferromagnetic barrier, and there is now an increasing amount of direct spectroscopic evidence [2] to test the existing theoretical models. In this talk we present scanning tunneling spectra of thin films of the ferromagnetic insulator europium sulfide on superconducting aluminum measured at 280 mK and in varying magnetic fields. We observe significant broadening of the superconducting energy gap and a variety of sub-gap structures induced by the presence of the ferromagnet. We interpret our findings based on the diffusive theory and a more advanced circuit theory model [3].

[1] F. S. Bergeret, Phys. Rev. Lett. 86, 4096 (2001)
[2] A. Di Bernardo, Nat. Comm. 6:8053 (2015)
[3] P. Machon, Phys. Rev. Lett. 110, 047002 (2013)

TT 14.4 Mon 15:45 HSZ 201

Thermoelectrical effects in hybrid superconducting Josephson junctions — •Alessandro Braggio[1,2,3], Riccardo Bosisio[1], Paolo Solinas[2], Sebastian Bergeret[4], and Francesco Giazotto[1] — [1]NEST, Istituto Nanoscienze-CNR, Piazza S. Silvestro 12, Pisa I-56127, Italy — [2]SPIN-CNR, Via Dodecaneso 33, 16146 Genova, Italy — [3]INFN, Sez. Genova, Via Dodecaneso 33, 16146 Genova, Italy — [4]Centro de Física de Materiales (CFM-MPC), Centro Mixto CSIC-UPV/EHU, Manuel de Lardizabal 4, E-20018 San Sebastián, Spain

We present an exhaustive theoretical analysis of charge and thermoelectric transport in a normal metal-ferromagnetic insulator-superconductor (NFIS) junction, and explore the possibility of its use as a sensitive thermometer. We evaluate the noise performance of open-circuit and closed-circuit setups. We show that temperature noise can be as low as 35nK $Hz^{-1/2}$[1]. In the second part we discuss the photon-mediated heat flow between two Josephson-coupled Bardeen-Cooper-Schrieffer (BCS) superconductors. We demonstrate that in standard low temperature experiments involving temperature-biased superconducting quantum interference devices (SQUIDs), this radiative contribution is negligible if compared to the direct galvanic one, but it largely exceeds the heat exchanged between electrons and the lattice phonons[2].

[1] F. Giazotto, P. Solinas, A. Braggio and F. S. Bergeret, Phys. Rev. Appl. 4, 044016 (2015)
[2] R. Bosisio, P. Solinas, A. Braggio and F. Giazotto, Phys. Rev. B 93, 144512 (2016)

TT 14.5 Mon 16:00 HSZ 201

Polarization dependence of the tunnel current in superconductor-ferroelectric-superconductor junctions — •Anke Sander, Victor Rouco, Laura Begon-Lours, Sophie Collin, Stephane Fusil, Jacobo Santamaría, Vincent Garcia, and Javier E. Villegas — Unité Mixte de Physique, CNRS, Thales, Univ. Paris-Sud, Université Paris Saclay, 91767 Palaiseau, France

In tunnel junctions with a ferroelectric barrier, a large resistance variation is observed upon ferroelectric switching, which can be induced by a short voltage pulse. Known as electroresistance, this phenomenon is connected to the interfacial screening of the electric field generated by the ferroelectric in the junction's electrodes.
Usually realized in junctions with normal-metal electrodes, here we experimentally investigate these effects in junctions that combine the ferroelectric $BiFeO_3$ and different types of superconducting electrodes. Using piezoresponse force microscopy and electrical measurements, we find an unusual temperature dependence of the electroresistance, which reaches up to 10^4% .The effects are discussed in terms of the interface charge-carrier depletion produced in the superconducting electrodes.

15 min. break.

Invited Talk TT 14.6 Mon 16:30 HSZ 201

Multi-Terminal Josephson Junctions as Topological Matter — •Julia S. Meyer — INAC/PHELIQS, Univ. Grenoble Alpes & CEA Grenoble, France

Topological phases of matter have attracted much interest in recent years. Starting with gapped phases such as topological insulators and superconductors, more recently gapless topological phases possessing topologically protected band crossings have been discovered.

We show that n-terminal Josephson junctions with conventional superconductors may provide a straightforward realization of tunable topological materials in n-1 dimensions [1], the independent superconducting phases playing the role of quasi-momenta. In particular, we find zero-energy Weyl singularities in the Andreev bound state spectrum of 4-terminal junctions.

Furthermore, we show that the presence of such Weyl singularities has important consequences on transport. Namely, it enables topological transitions that manifest themselves experimentally as changes of the quantized transconductance in units of $4e^2/h$ between two voltage-biased terminals.

[1] R.-P. Riwar, M. Houzet, J. S. Meyer, and Y. V. Nazarov, Nature Communications 7, 11167 (2016)

TT 14.7 Mon 17:00 HSZ 201

Multiple charge transport in a superconducting SET — •Thomas Lorenz, Susanne Sprenger, and Elke Scheer — University of Konstanz, 78467 Konstanz, Germany

A small island connected by two tunnel junctions forms a single electron transistor (SET) that shows Coulomb Blockade (CB) effects. The Orthodox Theory [1,2] quantitatively describes the behaviour in the weak-coupling regime, even in the case of superconducting transport. Despite much effort the transition from the weak- to the strong-coupling regime, in particular in the superconducting state, is not yet fully understood.

We are investigating transport through an all superconducting SET formed by an AlO_x tunnel barrier ($R_T \approx 120k\Omega$) and a mechanically controlled break junction (MCBJ). The MCBJ can be adjusted to cover the whole range from the tunneling (weak coupling) regime to the point-contact (strong coupling) regime. We discuss the interplay between the CB and the appearance of superconducting multiple charge transport (multiple Andreev reflection, Josephson effect).

[1] R. J. Fitzgerald, Phys. Rev. B 57, R11073(R) (1997).
[2] K. K. Likharev, Proc. IEEE 87, 606 (1999).

TT 14.8 Mon 17:15 HSZ 201

Nonequilibrium effects in hybrid superconducting turnstiles — •Ivan Khaymovich — Max Planck Institute for Physics of Complex Systems, Dresden, Germany

Many superconducting micro- and nano-electronic devices operating at low temperatures suffer from the presence of non-equilibrium quasiparticles. The number of these quasiparticles increases rapidly with the increase in the operation frequencies above the threshold determined by the relaxation rate. Slowing down of the relaxation rate at low temperatures conflicts, thus, the performance of modern cryoelectronic devices such as qubit systems, superconducting resonators, turnstiles, and superconducting hybrid electron coolers.

In this project on the example of single-electron sources we present both new types of such devices immune to the quasiparticle poisoning and methods of effective control of excess quasiparticles in such single electronic systems, based on the quasiparticle trapping and untrapping by the magnetic field an its interplay with the inverse proximity effect. Most of theoretical predictions have been experimentally verified and the theory is in good agreement with experimental data.

[1] I. M. Khaymovich et al., Phys. Rev. B 92, 020501(R) (2015)
[2] M. Taupin, I. M. Khaymovich et al., Nat. Comm. 7: 10977 (2016)
[3] D. M. T. van Zanten et al., Phys. Rev. Lett. 116, 166801 (2016)
[4] I. M. Khaymovich, D. M. Basko, Phys. Rev. B 94, 165158 (2016)
[5] S. Nakamura et al., in preparation

TT 14.9 Mon 17:30 HSZ 201

Double quantum dot Cooper-pair splitter at finite couplings — •Robert Hussein[1,2], Lina Jaurigue[3], Michele Governale[3], and Alessandro Braggio[2,4] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]SPIN-CNR, Via Dodecaneso 33, 16146 Genova, Italy — [3]School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology,Victoria University of Wellington, P.O. Box 600, Wellington 6140, New Zealand — [4]NEST, Istituto Nanoscienze-CNR, Piazza S. Silvestro 12, Pisa I-56127, Italy

We investigate the sub-gap physics of a Cooper-pair splitter based on a double quantum dot realized in a semiconducting nanowire. We study how the transport properties are determined by the interplay between local and nonlocal tunneling processes between the superconductor and the quantum dots. In the presence of interdot tunneling the system provides a simple mechanism to generate nonlocal entanglement even in the absence of nonlocal coupling with the superconducting lead. We show that spin-orbit interaction in combination with finite Coulomb energy opens the possibility to control the symmetry (singlet or triplet) of nonlocally entangled electron pairs.

[1] R. Hussein, L. Jaurigue, M. Governale, and A. Braggio, arXiv:1608.00504, accepted in Phys. Rev. B.

TT 14.10 Mon 17:45 HSZ 201

Theory of enhanced interlayer tunneling in optically driven high T_c superconductors — •Junichi Okamoto[1,2], Andrea Cavalleri[3,4], and Ludwig Mathey[1,2] — [1]Zentrum für Optische Quantentechnologien and Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany — [4]Department of Physics, Clarendon Laboratory, University of Oxford, Oxford OX1 3PU, United Kingdom

Motivated by recent pump-probe experiments indicating enhanced coherent c-axis transport in underdoped YBCO [1], we investigate Josephson junctions periodically driven by optical pulses [2]. We propose a mechanism for this observation by showing that a parametrically driven Josephson junction exhibits an enhanced imaginary part of the low-frequency conductivity when the driving frequency is blue-detuned to the plasma frequency, implying an effectively enhanced Josephson coupling. We show that the emergent driven steady state is a genuine, non-equilibrium superconducting state, in which equilibrium relations between the Josephson coupling, current fluctuations, and the critical current no longer hold. Transient response under a short pump pulse is also discussed to fully compare our theory with the experimental results.

[1] W. Hu et al., Nature Materials 13, 705 (2014)
[2] J. Okamoto, A. Cavalleri, L. Mathey, Phys. Rev. Lett. 117, 227001 (2016)

TT 14.11 Mon 18:00 HSZ 201

Josephson currents induced by the Witten effect — •Flavio Nogueira[1], Jeroen van den Brink[2], and Zohar Nussinov[3] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum — [2]Institute for Theoretical Solid State Physics, IFW Dresden — [3]Physics Department, CB 1105, Washington University

We reveal the existence of a new type of topological Josephson effect involving type II superconductors and three-dimensional topological insulators as tunnel junctions. We predict that vortex lines induce a variant of the Witten effect that is the consequence of the axion electromagnetic response of the topological insulator: at the interface of the junction each flux quantum attains a fractional electrical charge of $e/4$. As a consequence, if an external magnetic field is applied perpendicular to the junction, the Witten effect induces an AC Josephson effect in absence of any external voltage. We derive a number of further experimental consequences and propose potential setups where these quantized, flux induced, Witten effects may be observed.

[1] F. S. Nogueira, Z. Nussinov, and J. van den Brink, Phys. Rev. Lett. **117**, 167002 (2016)
[2] F. S. Nogueira, Z. Nussinov, and J. van den Brink, Phys. Rev. D **94**, 085003 (2016)

TT 15: Transport: Graphene and Carbon Nanostructures (jointly with DY, DS, HL, MA, O)

Time: Monday 15:00–18:15 Location: HSZ 204

TT 15.1 Mon 15:00 HSZ 204

Creating and steering highly directional electron beams in graphene — Ming-Hao Liu[1,2], •Cosimo Gorini[1], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, Regensburg, Germany — [2]Department of Physics, National Cheng Kung University, Tainan, Taiwan

We put forward a concept to create highly collimated, non-dispersive electron beams in pseudo-relativistic Dirac materials such as graphene or topological insulator surfaces [1]. Combining negative refraction and Klein collimation at a parabolic *pn* junction, the proposed lens generates beams, as narrow as a few Fermi wave lengths, that stay focused over scales of several microns and can be steered by a magnetic field without losing collimation. We demonstrate the lens capabilities by applying it to two paradigmatic settings of graphene electron optics: We propose a setup for observing high-resolution angle-dependent Klein tunneling, and, exploiting the intimate quantum-to-classical correspondence of these focused electron waves, we consider high-fidelity transverse magnetic focusing accompanied by simulations for current mapping through scanning gate microscopy. Our proposal opens up new perspectives for next-generation graphene electron optics experiments.

[1] M.-H. Liu, C. Gorini, K. Richter, arXiv:1608.01730.

TT 15.2 Mon 15:15 HSZ 204

Graphene *p-n* junction in a magnetic field as a valley switch — •Tibor Sekera, Rakesh P. Tiwari, and Christoph Bruder — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Low-energy excitations in graphene exhibit relativistic properties due to the linear dispersion relation close to the Dirac points in the first Brillouin zone. Two of the cones located at opposite corners of the first Brillouin zone can be chosen as inequivalent, representing a new *valley* degree of freedom, in addition to the charge and spin of an electron. Using the valley degree of freedom to encode information aroused significant interest, both theoretically and experimentally, and gave rise to the field of *valleytronics*.

We study a graphene *p-n* junction in an out-of-plane magnetic field as a platform to generate and controllably manipulate the valley polarization of electrons. We show that by tuning the external potential giving rise to the *p-n* junction we can switch the current from one valley polarization to the other. We also consider the effect of different types of edge terminations and present a setup, where we can partition an incoming valley-unpolarized current into two branches of valley-polarized currents. The branching ratio can be chosen by changing the location of the *p-n* junction.

TT 15.3 Mon 15:30 HSZ 204

Probing electronic wave functions in a nanotube quantum dot via conductance in a magnetic field — Magdalena Marganska[1], Alois Dirnaichner[1,2], Daniel R. Schmid[2], Peter L. Stiller[2], Christoph Strunk[2], Milena Grifoni[1], and •Andreas K. Hüttel[2] — [1]Institute for Theoretical Physics, Universität Regensburg, Regensburg, Germany — [2]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

The tunneling of electrons through a contact between two systems depends on the overlap of their electronic wave functions. In quantum dots the overlap is often tuned via the height of tunneling barriers. Conversely, in carbon nanotubes the unique combination of cylindrical topology and honeycomb atomic lattice allows for a manipulation of the longitudinal component of the electronic wave function via a parallel magnetic field. The amplitude of the wave function at the point of contact with the leads is directly reflected in the coupling strength. Experimentally, we detect the changes in the electronic wave function through the evolution of conductance resonances corresponding to single particle quantum states with magnetic field. The magnitude of the magnetic field in our experiment, up to 17 T, allows us to confirm our prediction of the very different behaviour of the two valley states. The K' valley states experience a strengthening of the tunnel coupling at low magnetic field, followed by subsequent decoupling. In contrast, the K valley states decouple from the leads monotonically, and coupling becomes unmeasurably small already for moderate magnetic fields.

TT 15.4 Mon 15:45 HSZ 204

Electron-electron interaction correction to tunneling in graphene-graphene nanojunctions — •Matthias Popp, Ferdinand Kisslinger, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg (FAU), Erlangen, Germany.

In weakly disordered conductors, electron-electron interaction is expected to provide a zero-bias anomaly in tunneling characteristics [1]. This purely electronic effect is seemingly suppressed in scanning tunneling spectroscopy experiments on graphene due to momentum mismatch, which requires phonon assisted tunneling. [2,3]. In order to overcome this limitation, we fabricate in-plane graphene-graphene nanojunctions by an electro burning process using epitaxial graphene on SiC as starting material. In some junctions with an overall conductance of about e^2/h we indeed observed a zero-bias anomaly at low temperatures which follows the logarithmic scaling characteristics predicted by *Altshuler* and *Aronov*. These experiments offer the opportunity to study the nonlocal aspects of electron tunneling via manipulation of the environment.

[1] Altshuler, B. L. and Aronov, A. G., *Electron-Electron Interaction in Disordered Conductors*, 1985
[2] Brar, V. W. et al., Applied Physics Letters, 2007, 91, 122102
[3] Zhang, Y. et al., Nature Physics, 2008, 4, 627-630

TT 15.5 Mon 16:00 HSZ 204

Electroluminescence of Graphene Nanojunctions — •Christian Ott, Konrad Ullmann, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstr. 7/A3, D-91058 Erlangen, Germany

We report on electroluminescence (EL) detected at graphene nanojunctions, the latter being formed by electroburning of epitaxial graphene ribbons on silicon carbide [1]. The EL shows a broad spectrum with emphasis on the near infrared regime. Its intensity scales with applied current and is temperature independent down to liquid helium temperatures. Surprisingly, we find a weak voltage dependence. The spectrum is similar to blackbody radiation with apparent temperatures well above the damage threshold of graphene and the silicon carbide substrate. A similar phenomenon has already been observed in single atom point contacts [2] and island metal films [3]. There a model was proposed based on hot electron luminescence which goes along with a large mismatch between electron gas temperature and lattice temperature due to a reduced electron-phonon interaction in nanoscopic structures. A critical discussion of the underlying mechanism is provided.

[1] Ullmann et al, Nano Letters 15, 5 (2015)
[2] Downes et al., Applied Physics Letters 81, 7 (2002)
[3] Fedorovich et al., Physics Reports 328 (2000)

TT 15.6 Mon 16:15 HSZ 204

Reversible Photochemical Control of Doping Levels in Supported Graphene — •Marie-Luise Braatz[1,2], Nils Richter[1,2], Hai I. Wang[1], Axel Binder[3], Mischa Bonn[4], and Mathias Kläui[1,2] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz (MAINZ), 55128 Mainz, Germany — [3]BASF SE, 67056 Ludwigshafen, Germany — [4]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

The type and density of carriers in graphene are important parameters to control its properties. Based on Terahertz (THz)-spectroscopy and electrical characterization of Nitrogen-doped graphene, we show that the doping level can be optically tuned between the p-type and intrinsic n-type regime [1]. This is achieved photochemically by controlling the dynamical equilibrium between the oxygen adsorption and desorption process via UV laser pulse irradiation treatment [2]. This approach is reversible, easy to use and contact free. This simple method can be used to write doping structures with spatial control by a focused laser beam, not requiring sophisticated nanostructuring to generate doping for instance by gate electrodes that need to be defined at the time of device fabrication.

[1] H. I. Wang, M.-L. Braatz et al., submitted (2016)
[2] S. M. Hornett et al., Phys Rev B 90 (2014)

15 min. break.

TT 15.7 Mon 16:45 HSZ 204

Time evolution of Floquet states in graphene — •Matteo Puviani[1], Francesco Lenzini[1], and Franca Manghi[1,2] — [1]Dipartimento FIM, Università di Modena e Reggio Emilia — [2]CNR - Institute of NanoSciences - S3, Modena

When a time-periodic field is applied to electrons in a lattice the Bloch theorem can be applied twice, both in space and in time, to describe the photon-dressed quasiparticles which are formed. This is the essence of Floquet theory, which has recently attracted a large renewed interest for its ability to describe topological phases in driven quantum systems. The discovery that circularly polarized light may induce nontrivial topological behavior in materials which would be standard in static condition has opened the way to the realization of the so-called Floquet Topological Insulators. In these systems, the topological phases may be engineered and manipulated by tunable controls such as polarization, periodicity and amplitude of the external perturbation.

In the presence of a continuous time-periodic driving, electrons are in a non-equilibrium steady state characterized by a time-periodic dependence of the wave function, and therefore of the expectation values of any observable. In this talk we will consider the prototypical case of graphene that, under the influence of circularly polarized light, exhibits in its Floquet band structure the distinctive features of a topological insulator, namely a gap in 2D and linear dispersive edge states in 1D (graphene nanoribbon). In particular, we will discuss how these characteristics affect the time behavior of some relevant observables such as energy, charge and current density.

TT 15.8 Mon 17:00 HSZ 204

Quantum chaos and out-of-time order correlation functions in graphene — •Markus Klug, Mathias Scheurer, and Jörg Schmalian — Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Deutschland

Out-of-time order correlation functions of type $C = \langle A(t)B(0)A(t)B(0)\rangle_\beta$ are believed to be a reasonable measure of quantum chaos which manifests in an exponential growth of C with a certain Lyapunov exponent determined by the microscopic model under considerations. Recently, it was conjectured hat this Lyapunov exponent is be bounded by $\lambda \leq 2\pi k_B T/\hbar$ [1].

In this work we investigate the out-of-time order correlation functions in graphene subject to the long range Coulomb interaction. To this end we develop a formalism to capture the relevant effects which determines the dominant time dependence of C. We demonstrate that the critical Dirac fluid graphene is a good candidate for saturating the bound mentioned above.

[1] J. Maldacena, S.H. Shenker and D. J. Stanford, High Energ. Phys. (2016) 2016: 106.

TT 15.9 Mon 17:15 HSZ 204

Interaction induced Dirac fermions from quadratic band touching in bilayer graphene — •Thomas C. Lang[1], Sumiran Pujari[2], Ganpathy Murthy[2], and Ribhu K. Kaul[2] — [1]Institute for Theoretical Physics, University of Innsbruck, Austria — [2]Department of Physics & Astronomy, University of Kentucky, Lexington, KY

We revisit the effect of local interactions on the quadratic band touching (QBT) of Bernal stacked bilayer graphene models using renormalization group (RG) arguments and quantum Monte Carlo simulations of the Hubbard model. We present an RG argument which predicts, contrary to previous studies, that weak interactions do not flow to strong coupling even if the free dispersion has a QBT. Instead they generate a linear term in the dispersion, which causes the interactions to flow back to weak coupling. Consistent with this RG scenario, in unbiased quantum Monte Carlo simulations of the Hubbard model we find compelling evidence that antiferromagnetism turns on at a finite U/t, despite the $U = 0$ hopping problem having a QBT. The onset of antiferromagnetism takes place at a continuous transition which is consistent with $z = 1$ as expected for Gross-Neveu criticality. We conclude that generically in models of bilayer graphene, even if the free dispersion has a QBT, small local interactions generate a Dirac phase with no symmetry breaking and there is a finite-coupling phase transition out of this phase to a symmetry-broken state.

TT 15.10 Mon 17:30 HSZ 204

Dynamical charge and pseudospin currents in graphene and possible Cooper pair formation — •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

With the quantum kinetic equations for systems with SU(2) structure, regularization-free density and pseudospin currents are calculated in graphene realized as the infinite mass-limit of electrons with quadratic dispersion and a proper spin-orbit coupling. The intraband and interband conductivities are discussed with respect to magnetic fields and magnetic domain puddles. The optical conductivity agrees well with the experimental values using screened impurity scattering and an effective Zeeman field. The universal value of Hall conductivity is shown to be modified due to this Zeeman field. The pseudospin current reveals an anomaly since a quasiparticle part appears though it vanishes for particle currents. The density and pseudospin response functions to an external electric field are calculated and the dielectric function is discussed with respect to collective excitations. A frequency and wave-vector range is identified where the dielectric function changes sign and the repulsive Coulomb potential becomes effectively attractive allowing for Cooper pairing.

[1] Phys. Rev. **B 94** (2016) 165415

TT 15.11 Mon 17:45 HSZ 204

Interplay between the long-range Coulomb interaction and edge-state magnetism in zigzag graphene nanoribbons — •Marcin Raczkowski and Fakher Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Quasi-one-dimensional graphene nanoribbons terminated by zigzag edges host partially flat bands at the Fermi energy. Theoretical studies of the Hubbard model with the effective on-site interaction only predict spontaneously induced spin polarizations at the zigzag edges and the associated finite dispersion of the low-energy band. Here, we revisit the stability and dynamical signatures of spin-polarized edge states by performing projective quantum Monte Carlo simulations of a more realistic model with long-range Coulomb interactions. On the one hand, increasing the relative strength of nonlocal interactions with respect to the on-site repulsion reduces noticeably the spin correlation length along the zigzag edge; nevertheless the tendency towards the extended spin polarization along the edges remains dominant over the competing short-range charge correlations. On the other hand, growing charge fluctuations are responsible for the emergence of incoherent low-energy excitations in the dynamical charge structure factor. In addition, we resolve a systematic shift of the dominant low-energy peak in single-particle spectral function on the edge towards higher frequencies that we attribute to quasiparticle scattering from charge excitations.

TT 15.12 Mon 18:00 HSZ 204

Quantum phase transition in effective spin ladders derived from graphene nanoribbons — •Cornelie Koop and Stefan Wessel — Institut für Theoretische Festkörperphysik, RWTH Aachen University

Zigzag edges of graphene nanoribbons host localized edge states, which show a ferromagnetic coupling along each edge and an antiferromagnetic one to the opposite edge. Using an effective model that treats the edge-bulk interaction as a perturbation to the edge-edge interaction, we can drastically reduce the numerical effort needed for this system, and we eventually find a rather general spin ladder model.

We examine this model at low, but finite temperatures by means of Monte-Carlo techniques using the stochastic series expansion method. Susceptibilities and correlation functions can be investigated. We find a quantum-phase transition (QPT), as a function of the antiferromagnetic inter-leg coupling strength, between a weak-coupling phase with long-range ferromagnetic order along each leg, which does not have a spin excitation gap, and a disordered, gapped singlet-phase. The location and estimates for the critical exponents are assessed by numerical methods and compared to known results from renormalization group calculations.

TT 16: Transport: Topological Phases (jointly with DS, MA, HL, O)

Time: Monday 15:00–18:00 Location: HSZ 304

TT 16.1 Mon 15:00 HSZ 304

Dynamical Buildup of a Quantized Hall Response from Non-Topological States — Ying Hu[1], Peter Zoller[1,2], and •Jan Carl Budich[3] — [1]Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, 6020 Innsbruck, Austria — [2]Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria — [3]Department of Physics, University of Gothenburg, SE 412 96 Gothenburg, Sweden

We consider a two-dimensional system initialized in a topologically trivial state before its Hamiltonian is ramped through a phase transition into a Chern insulator regime. This scenario is motivated by current experiments with ultracold atomic gases aimed at realizing time-dependent dynamics in topological insulators. Our main findings are twofold. First, considering coherent dynamics, the non-equilibrium Hall response is found to approach a topologically quantized time averaged value in the limit of slow but non-adiabatic parameter ramps, even though the Chern number of the state remains trivial. Second, adding dephasing, the destruction of quantum coherence is found to stabilize this Hall response, while the Chern number generically becomes undefined. We provide a geometric picture of this phenomenology in terms of the time-dependent Berry curvature.

TT 16.2 Mon 15:15 HSZ 304

Sign reversal of the quantized topological Hall effect in skyrmion crystals — •Börge Göbel[1], Alexander Mook[1], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — [2]Institut für Physik, Martin-Luther-Universität, D-06120 Halle

The topological Hall effect (THE) of electrons [1] is the hallmark of a skyrmion crystal phase [2]. It can be understood either by coupling of the electrons' spin to the local magnetic texture (Zeeman interaction) or by coupling of the electrons' charge to the emergent field generated by the texture (Peierls substitution).

Here, we study the THE on a triangular lattice, addressing band structure, Hall conductivity, and topological surface states. In this system, the THE is quantized and the transverse conductivity changes sign if the Fermi energy crosses a van Hove singularity. By mapping the THE to a quantum Hall effect (QHE) on a lattice [3], we assign this prominent feature to the cyclotron mass of electron orbits, that is, when constant-energy cuts of the band structure change from electron to hole pockets. Based on this picture, we derive an approximate rule which allows to determine the energy dependence of the topological Hall conductivity in *any* two-dimensional lattice.

[1] K. Hamamoto et al., Phys. Rev. B **92**, 115417 (2015)
[2] S. Mühlbauer et al., Science **323**, 915 (2009)
[3] Y. Hatsugai et al., Phys. Rev. B **74**, 205414 (2006)

TT 16.3 Mon 15:30 HSZ 304

Edge states and topology in finite-length single-wall carbon nanotubes — •Wataru Izumida[1,2], Rin Okuyama[3], Ai Yamakage[4,5], Mikio Eto[3], and Riichiro Saito[1] — [1]Department of Physics, Tohoku University, Sendai 980-8578, Japan — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [3]Faculty of Science and Technology, Keio University, Yokohama 223-8522, Japan — [4]Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan — [5]Institute for Advanced Research, Nagoya University, Nagoya 464-8601, Japan

Edge states in finite-length single-wall carbon nanotubes, which appear in the energy gap of the bulk states, are studied from the topological viewpoint [1,2]. An effective one-dimensional (1D) lattice model is introduced to analyze the quantum system with boundary. By analyzing the 1D lattice model, a bulk-edge correspondence, relationship between the number of edge states in the energy gap and the topological winding number defined in the corresponding bulk system, is given [1]. Manipulation of the edge states by magnetic field [3,4] is suggested in terms of the topological phase transition [2].

[1] W. Izumida, R. Okuyama, A. Yamakage, R. Saito, Phys. Rev. B 93, 195442 (2016).
[2] R. Okuyama, W. Izumida, M. Eto, arXiv:1610.05034.
[3] K. Sasaki, S. Murakami, R. Saito, Y. Kawazoe, Phys. Rev. B 71, 195401 (2005).
[4] M. Marganska, M. del Valle, S. H. Jhang, C. Strunk, M. Grifoni, Phys. Rev. B 83, 193407 (2011).

TT 16.4 Mon 15:45 HSZ 304

Topological invariants in carbon nanotubes with superconducting pairing — •Lars Milz[1], Magdalena Marganska[1], Wataru Izumida[1,2], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93 047 Regensburg, Germany — [2]Department of Physics, Tohoku University, Sendai 980-8578, Japan

The symmetries present in a gapped Hamiltonian system determine the types of topological invariants which can be defined for that system. Our case of interest here is a carbon nanotube, which in its normal state is known to possess a non-trivial integer topological invariant, the winding number. Its value determines the number of edge states. When a superconducting pairing is imposed on the nanotube, the symmetry class of the system changes and it is possible to define also a Z2 Pfaffian topological invariant, exploiting the particle-hole rather than the chiral symmetry. We explore the relationship between the two invariants and their influence on the energy spectrum and eigenstates, in particular the edge modes, of a finite carbon nanotube.

TT 16.5 Mon 16:00 HSZ 304

Renormalization group approach to topological phase transitions — •Wei Chen[1], Manfred Sigrist[1], and Andreas Schnyder[2] — [1]ETH Zurich, Zurich, Switzerland — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Have you thought about this: every time you tie your shoelaces, you are using a scaling procedure (the tying) to make the topology (the knot) more obvious? Akin to knot-tying, a renormalization group approach is proposed to judge topological phase transitions for systems that belong to any dimension and symmetry class, and whether the topological phase transition is driven by noninteracting parameters (hopping, chemical potential, etc) as in the usual topological insulators, or interacting parameters (Hubbard interaction, etc) as in fractional Chern insulators. The meaning of scale invariance at the critical point and the fixed point is shown to be related to the notion of correlation length, which was previously thought to be nonexistent for topological insulators.

[1] W. Chen, J. Phys. Condens. Matter 28, 055601 (2016)
[2] W. Chen, M. Sigrist, and A. P. Schnyder, J. Phys. Condens. Matter 28, 365501 (2016)

TT 16.6 Mon 16:15 HSZ 304

Fermionic topological quantum states as tensor networks — •Carolin Wille, Oliver Buerschaper, and Jens Eisert — Institut für theoretische Physik, Freie Universität Berlin

Tensor network states, and in particular projected entangled pair states, play an important role in the description of strongly correlated quantum lattice systems. They do not only serve as variational states in numerical simulation methods, but also provide a framework for classifying phases of quantum matter and capture notions of topological order in a stringent and rigorous language. The rapid development in this field for spin models and bosonic systems has not yet been mirrored by an analogous development for fermionic models. In this work, we introduce a tensor network formalism capable of capturing notions of topological order for quantum systems with fermionic components. At the heart of the formalism are axioms of fermionic matrix product operator injectivity, stable under concatenation. Building upon that, we formulate a Grassmann number tensor network ansatz for the ground state of fermionic twisted quantum double models. A specific focus is put on the paradigmatic example of the fermionic toric code. This work shows that the program of describing topologically ordered systems using tensor networks carries over to fermionic models.

15 min. break.

TT 16.7 Mon 16:45 HSZ 304

Finite-size scaling around a topological phase transition — •Tobias Gulden[1,2], Yuting Wang[2], and Alex Kamenev[2] — [1]Technion - Israel Institute of Technology — [2]University of Minnesota

The critical point of a phase transition is described by a conformal field theory, where perturbations away from criticality are known to give rise

to universal scaling functions. We consider perturbations around a critical point which separates two distinct topological phases. For both energy and entropy we find the existence of scaling functions which depend on the sign of the perturbation, i.e. they discriminate between topological phases. Renyi entropy of the Kitaev model contains two distinct scaling functions which separate a well-known universal part and the topological contribution, while energy has one asymmetric scaling function. The latter is universal for all five Altland-Zirnbauer symmetry classes with non-trivial topology in one spatial dimension.

TT 16.8 Mon 17:00 HSZ 304

Fractionalization of charge and energy after electron injection in 1D helical systems — •Alessio Calzona[1,2,3], Matteo Acciai[1], Matteo Carrega[4], Fabio Cavaliere[1,3], and Maura Sassetti[1,3] — [1]University of Genova, Italy — [2]University of Luxembourg, Luxembourg — [3]SPIN-CNR, Genova, Italy — [4]NEST, Pisa, Italy

The possibility to inject a single electron into ballistic 1D conductors is at the basis of the new and fast developing field of electron quantum optics. In this respect, helical edge states of topological insulators can be used as electronic waveguides and would be an ideal playground [1,2].

Here we thus study and characterize the tunneling of a single electron from a mesoscopic capacitor into a couple of interacting helical edge channels [3]. The injection process leads to the creation of a pair of fractional excitations travelling in opposite directions. Their charge and energy profiles are analyzed. We also show that the energy partitioning between the two fractional excitations depends both on the interaction strength and on the injection parameters. Interestingly, this allows for a situation in which energy and charge mainly flow in opposite directions. In addition, such peculiar behavior of energy partitioning suggests that it can be also used as a tool to probe features of out-of-equilibrium systems [4].

[1] G. Fève et al., Science 316, 1169 (2007)
[2] D. Ferraro et al., PRB 89, 075407 (2014)
[3] A. Calzona et al., PRB 94, 035404 (2016)
[4] A. Calzona et al., arXiv:1610.04492

TT 16.9 Mon 17:15 HSZ 304

Solitons in one-dimensional lattices with a flat band — •Dario Bercioux[1,2], Omjyotu Dutta[1], and Enrique Rico[2,3] — [1]Donostia International Physics Center (DIPC), E-20018 San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation for Science, Maria Diaz de Haro 3, 48013 Bilbao, Spain — [3]Department of Physical Chemistry, University of the Basque Country UPV/EHU, Apartado 644, E-48080 Bilbao, Spain

We investigate the spectral properties of a quasi-one-dimensional lattices in two possible dimerization configurations [1]. Both configurations are characterized by the same lattice topology and the same spectra containing a flat band at zero energy. We find that, one of the dimerized configuration has similar symmetry to an one-dimensional chain proposed by Su-Schrieffer-Heeger [2] for studying solitons in conjugated polymers. Whereas, the other dimerized configuration only shows non-trivial topological properties in the presence of chiral-symmetry breaking adiabatic pumping.

[1] D. Bercioux, O. Dutta & E. Rico, arXiv:1609.06292.
[2] W. P. Su, J. R. Schrieffer, & A. J. Heeger Phys. Rev. Lett. **42**, 1698 (1979).

TT 16.10 Mon 17:30 HSZ 304

Local nature of Quantized Hall Effect — •Afif Siddiki — Mimar Sinan Fine Arts University, Physics Department, Sisli-Istanbul, Turkey 34380

Here, we investigate the electrostatic properties of two dimensional electron system (2DES) in the integer quantum Hall regime. As it is well known, the Landau quantization emerges from strong perpendicular magnetic fields. The (Landau) energy levels are broadened due to impurities, which we embedded their effects in density of states (DOS). As a simple model, DOS have two different forms: the Gaussian and semi-elliptic descriptions, i.e. the self consistent Born approximation (SCBA). Having in hand DOS, we obtain both the longitudinal and Hall (transversal) conductivities (σ_L, σ_H) utilizing Thomas-Fermi-Poisson approximation to calculate the charge density profile and Drude model to obtain transport coefficients. Since, the definition of capacitance is closely related with compressibility, (local) screening properties of 2DES is extremely important. Here we numerically simulate a translational invariant Hall bar subject to high magnetic fields which is perpendicular to the plane of the 2DES using realistic parameters extracted from the related experiments. Using the above mentioned approaches the local capacitances are calculated, numerically. Our findings are in perfect agreement with the related experiment which is based on a dynamic scanning capacitance microscopy technique.

TT 16.11 Mon 17:45 HSZ 304

Properties of non-abelian hierarchy states in the fractional quantum Hall effect — •Yoran Tournois and Maria Hermanns — Institute for Theoretical Physics, Cologne, Germany

The fractional quantum Hall effect is one of the paradigmatic examples of topological order in condensed matter physics. While the physics of the fractional quantum Hall effect is well understood in the lowest Landau level by means of the Haldane-Halperin hierarchy, a general method to describe the properties of quantum Hall liquids in the second Landau level is lacking. These are of particular interest, as it is believed that they may harbor exotic excitations - non-abelian anyons. In this talk, we consider a general class of model wave functions, which were recently proposed as a generalization of the Haldane-Halperin hierarchy. While these are conjectured to describe non-abelian quantum Hall liquids, many of their properties are not manifest and thus previously unknown. We determine their properties using a variety of methods. In particular, we derive the explicit conformal field theory description of the model wave functions, which reveals the non-abelian braiding statistics of the quasiparticles as well as the edge theory.

TT 17: Magnetic Heuslers, Half-Metals and Oxides (joint session MA, TT, organized by MA)

Time: Monday 15:00–18:30 Location: HSZ 403

TT 17.1 Mon 15:00 HSZ 403

Giant anomalous Hall effect in Heusler compounds — •Kaustuv Manna[1], Rolf Stinshoff[1], Ting-Hui Kao[1], Nitesh Kumar[1], Chandra Shekhar[1], Jayita Nayak[1], Sunil Wilfred DSouza[1], Sanjay Singh[1], Gerhard H. Fecher[1], Stuart S. P. Parkin[2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany

The Co-Based Heusler compounds have drawn considerable interest in last few years for the spintronics application due to the prediction of large anomalous Hall effect (AHE) as well as spin Hall effect [1]. For many of the samples like Co_2MnAl, Co_2MnGa etc. formation of the Weyl points near Fermi energy was proposed to be the origin for such fascinating behaviour [2]. Here we report the giant anomalous Hall effect in Co_2MnGa single crystals. The sample crystallizes with $Fm\bar{3}m$ which hold the inversion symmetry and the AHE observed $\sim$ 1200 S cm^{-1} at 2 K. The ferromagnetic moment found $\sim$ 4.23 μ_B/fu. On the contrary, for the systems where the inversion symmetry is broken, like Mn_2CoGa [$F\bar{4}3m$], there is no Weyl point in the band structure. Interestingly we don't observe any AHE at 2 K though the system possess ferromagnetic moment of $\sim 2.27\ \mu_B/fu$.

[1]Jen-Chuan Tung and Guang-Yu Guo, New J. Phys. **15**, 033014 (2013).
[2]J. Kubler and C. Felser, Europhys. Lett. **114**, 47005 (2016).

TT 17.2 Mon 15:15 HSZ 403

Magnetic field assisted heat treatment — •Franziska Seifert[1], Bernd Büchner[1,2], and Sabine Wurmehl[1] — [1]Leibniz Institute for Solid State Research Dresden, Germany — [2]Technische Universität Dresden, Germany

The convetionell way to improve or tailor the structural and physical properties of a material is, in most of the cases, high temperature annealing. It is also possible to anneal the material at a certain magnetic field at room temperature. With our device we combine both, magnetic field and high temperature treatments. We are able to tai-

lor the magnetic properties by applying a magnetic field during high temperature annealing. Especially in multiphase materials, we can favour particular one phase, which determines the magnetic properties. This annealing technique is very interesting for shape memory alloys, magnetocaloric, hardmagnetic or highly spin polarized materials. Our preliminary results will be discussed.

TT 17.3 Mon 15:30 HSZ 403

Stability of a highly spin polarized surface resonance of Co_2MnSi at spin-valve interfaces — •Christian Lidig[1], Alexander Kronenberg[1], Andrei Gloskovskii[2], Mathias Kläui[1], and Martin Jourdan[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]Deutsches Elektronen-Synchrotron DESY, 22603 Hamburg, Germany

The magnitude of the spin polarization of ferromagnetic materials is a key property for their application in spin transport-based electronics. However it is not the bulk, but the interface of the material, which is relevant for applications. Investigating thin films of Co_2MnSi (CMS) by spin-resolved UPS and spin-integrated HAXPES, we recently observed a high spin polarization at room temperature in a wide energy range below the Fermi energy, which is related to a stable highly spin polarized surface resonance[1,2]. Correspondingly, CMS / Ag / CMS spin valves show large GMR values[3]. However, the use of alternative spacer layers like Cr[4] always resulted in strongly reduced GMR values. A characteristic spectral feature close to the Fermi edge in HAXPES is related to the surface resonance[1]. This spectral feature is completely suppressed at CMS interfaces with Al and Cr and diminished in combination with Cu. However, it is fully conserved at epitaxial interfaces with Ag, explaining the superior magnetoresistance of spin-valves with this materials combination. [1] M. Jourdan et al., Nat. Commun. **5**, 3974 (2014). [2] J. Braun et al., Phys. Rev. B **91**, 195128 (2015). [3] Y. Sakuraba et al., Appl. Phys. Lett. **101**, 252408 (2012). [4] K. Yakushiji et al. Appl. Phys. Lett. **88**, 222504 (2006).

TT 17.4 Mon 15:45 HSZ 403

Defect-induced magnetic structure of CuMnSb — •Frantisek Maca[1], Josef Kudrnovsky[1], Vaclav Drchal[1], and Ilja Turek[2] — [1]Institute of Physics ASCR, Praha, Czech Republic — [2]Charles University, Faculty of Mathematics and Physics, Praha, Czech Republic

We have investigated the magnetic phases of CuMnSb Heusler alloy with defects which exist in real experimental conditions. Total energy calculations confirm that the AFM[100]-phase is the ground state for the ideal CuMnSb in contrast to the experimentally observed AFM[111]-phase. Calculated formation energies indicate as possible candidates for defects the Cu-Mn swaps for the stoichiometric alloy and Mn-antisites on Cu-lattice and Mn-interstitials for Mn enriched alloys.

The total energies of various magnetic phases of CuMnSb with defects were determined using two different structural models, namely, the full-potential supercell approach and the alloy model employing the coherent potential approximation (CPA). We have found that the AFM[111]-ground state is stabilized for a low critical impurity concentrations approximately 3% . We have also investigated the influence of defects on the exchange interactions among Mn-moments and the stability of magnetic order by using the Heisenberg model Hamiltonian. The stability of the AFM[111] phase is in all cases enhanced by electron correlations in narrow Mn-bands treated here in the static limit (LDA+U).

TT 17.5 Mon 16:00 HSZ 403

Magnetotransport in Half-Metallic Manganese Ruthenium Gallium — •Ciaran Fowley[1], Kiril Borisov[2], Gwenael Atcheson[2], Yong-Chang Lau[2], Naganivetha Thiyagarajah[2], Rodolfo Gallardo[3], Jurgen Lindner[1], Zhaosheng Wang[4], Erik Kampert[4], Mike Coey[2], Plamen Stamenov[2], Karsten Rode[2], and Alina Maria Deac[1] — [1]Institute for Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Germany — [2]AMBER and School of Physics, Trinity College Dublin, Dublin 2, Ireland — [3]Universidad Técnica Federico Santa María, Valparaíso, Chile — [4]High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Germany

The recently discovered fully-compensated half-metal, manganese-ruthenium-gallium (MRG), is a very promising material for spintronics. It possesses tunable magnetic moment, high magnetic anisotropy field and high spin polarisation. Here, we use the extraordinary Hall effect and longitudinal magnetoresistance to characterise the properties of MRG. Experiments are carried out in pulsed magnetic fields up to 60 T at the Dresden High Magnetic Field Laboratory (HLD). The spin-flop transition, as well as a large spontaneous Hall angle (over 2%) is observed. The magneto-transport in MRG is shown to be dominated by one sublattice only. The spontaneous Hall angle is non-zero even at the magnetic compensation temperature (i.e. when the total magnetic moment is zero). MRG behaves magnetically like an antiferromagnet and electrically as a normal ferromagnet with a sizeable spin-polarisation.

TT 17.6 Mon 16:15 HSZ 403

Tunneling Magnetoresistance in MnRuGa based Magnetic Tunnel Junctions — •Aleksandra Titova[1,2], Ciaran Fowley[1], Kiril Borisov[3], Davide Betto[3], Yong Chang Lau[3], Nivetha Thiyagarajah[3], Gwenael Atcheson[3], Michael Coey[3], Plamen Stamenov[3], Karsten Rode[3], Jürgen Lindner[1], Jürgen Fassbender[1,2], and Alina Deac[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Technische Universität Dresden, Germany — [3]Trinity College, Dublin, Dublin, Ireland

Some intermetallic Heusler compounds display high spin polarization and low magnetic moment. Thin-film samples can possess huge uniaxial anisotropy fields, exceeding tens of teslas. This, combined with their tuneable properites, make these materials very attractive for THz based spin-transfer-torque oscillators. Recently new material from this family was discovered - MnRuGa (MRG) - the first experimentally achieved fully-compensated half-metallic ferrimagnet. Here we show that MRG can be integrated in perpendicular anisotropy magnetic tunnel junctions stacks. Tunneling magnetoresistance (TMR) ratios up to 40% are observed. We also demonstrate that the TMR exists even when the net magnetization of MRG is strictly zero, implying that, at compensation, MRG exhibits a sizable spin polarization. The role of different diffusion barrier layers between MRG and the tunneling barrier as well as annealing temperature was investigated.

This work is supported by the Helmholtz Young Investigator Initiative Grant No. VH-N6-1048.

15 min. break.

TT 17.7 Mon 16:45 HSZ 403

Influence of grain boundaries on cohesive and magnetic properties in the inverse Heusler phase Fe_2CoGa — •Georg Krugel, Daniel Urban, Wolfgang Körner, and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

Heusler phases are promising candidates in the search for a rare-earth free hard-magnetic compound allowing high Curie temperatures. Experimentally, they are often found to be brittle and the effect of their microstructure on the material properties is not yet understood in detail.

Using DFT calculations we investigate the effect of grain boundaries (GB) on the mechanical and magnetic properties of the inverse Heusler phase Fe_2CoGa as a case study. Four different GBs are studied and several different translation states taken into account for each of them to sample the gamma surface. The GB excess volume, the formation energy of the GB and the cohesion energies of the grains are calculated and compared in order to shed more light onto the influence of GB on the mechanical properties of Heusler phases. For an understanding of the behaviour of magnetism at the GB the local atomic configurations are analysed together with the atomic magnetic moments. Moreover, we calculate the magnetic anisotropy energies for the energetically most favorable configurations. Our results support experimental efforts to determine tailored synthesis routes.

TT 17.8 Mon 17:00 HSZ 403

Study of compensated ferrimagnetic Heusler materials $Mn_{3-x}Pt_xGa$ — •Vivek Kumar[1], Ajaya K. Nayak[1,2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

Compensated ferrimagnets with large spin polarization and high ordering temperature are perfect candidates for realization of antiferromagnetic spintronics. These materials with additional perpendicular magnetocrystalline anisotropy can be ideal candidates for spin transfer torque applications. In this direction Heusler materials find special attention where chemical disorder can be used as an engineering tool

to improve desired properties. The tetragonal Mn_3Ga is an interesting candidate as a starting material which exhibits a high Curie temperature (T_C). It is theoretically predicted that substitution of Mn with a late transition metal can lead to a decrease in the total magnetic moment [1]. Here we present the structural and magnetic properties of single phase bulk tetragonal $Mn_{3-x}Pt_xGa$ Heusler materials for x varying from 0 to 0.6. We have found that the tetragonal distortion increases with increasing Pt concentration, indicating stabilization of the tetragonal phase with Pt substitution. With increasing Pt concentration the total magnetic moment systematically decreases and reach a compensation point around x=0.6. Although the magnetic ordering temperature displays a slight reduction with Pt substitution the compensated sample exhibits a T_C well above room temperature.
[1]R. Sahoo *et al.*, Adv. Mat. **28**, 8499 (2016).

TT 17.9 Mon 17:15 HSZ 403

High quality Yttrium Iron Garnet thin films by room temperature deposition and annealing in argon atmosphere — •Christoph Hauser[1], Christian Eisenschmidt[1], Hakan Deniz[2], and Georg Schmidt[1,3] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [3]Interdisziplinäres Zentrum für Materialwissenschaften, Halle, Germany

We have recently [1] shown that depositing Yttrium Iron Garnet by Pulsed Laser Deposition at room temperature and subsequent annealing in an oxygen atmosphere results in fully epitaxial layers. The layers show extremely low damping and very narrow linewidth in Ferromagnetic Resonance, even for thin layers. Here we show that annealing in oxygen is not mandatory. Also annealing in argon results in high quality layers. For a 63 nm YIG layer a linewidth of 2.26 Oe @ 9.6GHz and a damping of $1.61 \cdot 10^{-4}$ is observed in FMR. Structural characterization indicates high crystalline quality and no visible defects. [1] Hauser *et al.*, Sci. Rep. 6, 20827 (2016)

TT 17.10 Mon 17:30 HSZ 403

Colossal increase in the magnetic moment of NiCo2O4 films via He-ion irradiation — •Parul Pandey[1], Yugandhar Bitla[2], Matthias Zschornak[1], Mao Wang[1], Chi Xu[1], Joerg Grenzer[1], Sibylle Gemming[1], Manfred Helm[1], Ying-Hao Chu[2,3], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum-Dresden -Rossendorf, Dresden, Germany — [2]National Chiao Tung University, Hsinchu, Taiwan — [3]Institute of Physics, Academia Sinica, Taipei, Taiwan

The spinel NiCo2O4 exhibits the unique combination of electrical conductivity, infrared transparency, electro catalytic activity, and ferrimagnetic order, which makes it an attractive material for spintronic applications. The NiCo2O4 thin-films electrical and magnetic properties can be manipulated from high temperature ferrimagnetic and metallic to low temperature ferromagnetic and insulating by changing the growth temperature. The high-quality epitaxial NiCo2O4 films were grown on MgAl2O4 (100) substrate at ~ 400°C exhibits metallic behavior accompanied by ferrimagnetic order with moment ~ 2 μB/fu. Here, we report the impact of He-ion irradiation with fluence ranging from 5*1015/cm2 - 3*1016/cm2 on these metallic NiCo2O4 films. The use of He-ion irradiation results in the coherent control of out-of-plane lattice parameter of these films without changing its in-plane lattice parameter. The comprehensive study of magnetization data reveals the magnetic moment in the irradiated films increases drastically to ~ 4 μB/fu. The X-ray absorption spectroscopic study also suggests the possible charge redistribution within the octahedral sites of the NiCo2O4 films which corroborate well with the increase in the magnetic moment.

TT 17.11 Mon 17:45 HSZ 403

Magnetic and structural properties in the spin-dimer system Ba0.1Sr2.9Cr2O8 — •Alsu Gazizulina[1], Diana Lucia Quintero Castro[2], and Andreas Schilling[1] — [1]Physik-Institut of University of Zurich, Zurich, Switzerland — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Sr3Cr2O8 and Ba3Cr2O8 are two insulating dimerizad antiferromagnets with the magnetic ions, Cr 5+, that lie on hexagonal bilayers with strong intradimer antiferromagnetic interaction. This leads to a singlet ground state and gapped triplet states. Intradimer interaction constant J0 strongly depends on the stoichiometry.

We report on the change of the structural and magnetic properties of a spin-dimer system, Sr3Cr2O8, by introducing chemical disorder. Two large single crystal of Ba(3-x)Sr(x)Cr2O8 with x=2.9 and x=2.8 have been grown in a four-mirror type optical floating-zone furnace. By performing magnetization, heat-capacity measurements we have studied structural and magnetic properties of these compounds. Our inelastic neutron scattering measurements of spin-dimer compound Ba0.1Sr2.9Cr2O8 determine the interaction constants and the spin gap. The intradimer interaction constant is found to be J0=5.327(1) meV, that about 8% smaller than for pure Sr3Cr2O8 compound. Spin gap is decreasing about 6% with introducing chemical disorder.

TT 17.12 Mon 18:00 HSZ 403

First principles study of orbital order in Mn doped FeV2O4 — Dibyendu Dey[1], •Tulika Maitra[2], and Arghya Taraphder[1] — [1]Department of Physics, Indian Institute of Technology, Kharagpur 721302, India — [2]Department of Physics, Indian Institute of Technology, Roorkee 247667, India

The long range orbital order in vanadium spinel oxides has been thoroughly debated by condensed matter physicists in recent years. MnV_2O_4 and FeV_2O_4 are two such compounds where the debate is centered around whether there are complex or real orbitals involved in the ordering process. In this context, we have investigated the long range orbital order in Mn doped FeV_2O_4 as a function of Mn doping (x). We have employed first-principles density functional theory (DFT) including Coulomb correlation (GGA+U) and spin-orbit interaction (GGA+U+SO) as well as the wannierization of our DFT derived vanadium d-bands for our analysis of the orbital order in these systems. We observe that for $x \leq 0.6$, the orbital order at V sites consists of a linear superposition of d_{xz} and d_{yz} orbitals of the type dxz±dyz whereas for $x > 0.6$, A-type ordering is observed. The effect of spin-orbit interaction on orbital ordering is found to be not significant in the entire range of doping studied indicating the absence of complex orbitals in the ordering[1]. We also analyze the orbital ordering from the Raman spectrum calculated using ab-initio phonon within the DFT framework and compare the same with the experimental observations.

Reference: [1] Dibyendu Dey, T. Maitra, and A. Taraphder; Phys. Rev. B 93, 195133 (2016)

TT 17.13 Mon 18:15 HSZ 403

Curie temperature of ultra-thin EuO films in proximity to a metal — Brian Tam, Andreas Reisner, Steffen Wirth, •Simone G. Altendorf, and Liu Hao Tjeng — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

A reduction of the thickness of ferromagnetic layers towards the ultra-thin limit goes along with a strong reduction of the Curie temperature thereby hindering potential technological applications. We study the possibility to compensate the lowering of the magnetic ordering temperature of ultra-thin EuO films by bringing them in close proximity to a metal, thereby trying to make use of the so-called image charge screening effect to increase the strength of the magnetic exchange interactions. We utilize the well-established Eu-distillation-assisted MBE growth method to prepare highly stoichiometric EuO films on YSZ substrates. By capping one half of each film with a Mg metal overlayer and the other half with MgO, we were able to directly determine the effectiveness of the proximity effect of the metal to influence the magnetic properties of ultra-thin ferromagnetic films.

TT 18: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - II (joint session DS, HL, MA, MM, O, TT, organized by O)

Time: Monday 15:00–18:15 Location: GER 38

Invited Talk TT 18.1 Mon 15:00 GER 38

Towards efficient orbital-dependent density functionals for weak and strong correlation — •Igor Ying Zhang[1], Patrick Rinke[1,2], John P. Perdew[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Aalto University, Finland — [3]Temple University, USA

We present a new paradigm for the design of exchange-correlation functionals in density-functional theory [1]. Electron pairs are correlated explicitly by means of the recently developed second order Bethe-Goldstone equation (BGE2) approach [2]. Here we propose a screened BGE2 (sBGE2) variant that efficiently regulates the coupling of a given electron pair. sBGE2 correctly dissociates H_2 and H_2^+, a problem that has been regarded as a great challenge in density-functional theory for a long time [3]. The sBGE2 functional is then taken as a building block for an orbital-dependent functional, termed ZRPS, which is a natural extension of the PBE0 hybrid functional. While worsening the good performance of sBGE2 in H_2 and H_2^+, ZRPS yields a remarkable and consistent improvement over other density functionals across various chemical environments from weak to strong correlation. [1] IY Zhang et al., Phys. Rev. Lett. 117, 133002 (2016); [2] IY Zhang et al., New J. Phys. 18 073026 (2016); [3] AJ Cohen et al., Chem. Rev. 112 289 (2011).

TT 18.2 Mon 15:30 GER 38

Towards a functional for strong correlation via semiclassical model for the indirect energy and local interpolation along the adiabatic connection — •Stefan Vuckovic and Paola Gori-Giorgi — Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling, FEW, Vrije Universiteit, De Boelelaan 1083, 1081HV Amsterdam, The Netherlands

Finding an approximate XC functional that is able to capture strong correlation effects is a big, unsolved DFT challenge. Even a bigger challenge is to find a functional able to treat any correlation regime successfully. We attempt to construct an XC functional that has no bias towards a particular correlation regime by using a local interpolation along the adiabatic connection between the weak and the strong coupling limit of DFT. [1] In addition to this approach, I will also present our semiclassical model for accurate indirect energies. I will discuss how this model can be used for a construction of XC functionals, exploiting its XC energy density in the conventional gauge, the one of the electrostatic potential of the XC hole.

1. Stefan Vuckovic, Tom J. P. Irons, Andreas Savin, Andrew M. Teale, and Paola Gori-Giorgi, Journal of Chemical Theory and Computation 2016, 12 (6), 2598-2610

TT 18.3 Mon 15:45 GER 38

Benchmark of *GW* approaches for the *GW*100 test set — •Patrick Rinke[1], Matthias Dauth[2], Fabio Caruso[3], and Michiel van Setten[4] — [1]COMP Centre of Excellence, Aalto University, Finland — [2]University of Bayreuth, Germany — [3]University of Oxford, England — [4]Université Catholique de Louvain, Belgium

Many-body theory in the *GW* approach has become the method of choice for calculating charged excitations in solids. Now it is increasingly being applied to molecules, but fundamental questions regarding its *modus operandi* and its accuracy remain. To address both of these aspects, we present a comprehensive assessment of different *GW* methodologies for the recent *GW*100 test set [1] of molecular ionization energies [2]. We compare our *GW* calculations to coupled-cluster singles, doubles, and perturbative triples [CCSD(T)] reference data for *GW*100. We find ionization energies of fully self-consistent *GW* and quasiparticle self-consistent *GW* in excellent agreement with CCSD(T), with discrepancies typically smaller than 0.3 eV and 0.2 eV, respectively. For partially self-consistent and perturbative *GW* the deviation from CCSD(T) is strongly dependent on the starting point. An optimal starting point is found by minimizing the deviation from the straight-line error [3], which concomitantly yields a systematic improvement of the ionization energies. [1] M. J. van Setten, P. Rinke, *et al.*, J. Chem. Theory Comput. **11**, 5665 (2015), [2] F. Caruso, M. Dauth, M. J. van Setten, and P. Rinke, J. Chem. Theory Comput. **12**, 5076 (2016), [3] M. Dauth, F. Caruso, S. Kümmel, and P. Rinke, Phys. Rev. B **93**, 121115(R) (2016).

TT 18.4 Mon 16:00 GER 38

Addressing electron-hole correlation in core excitations of solids: A first-principles all-electron approach based on many-body perturbation theory — •Christian Vorwerk, Caterina Cocchi, and Claudia Draxl — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

In the framework of an all-electron implementation of many-body perturbation theory, we investigate K, $L_{2,3}$, and M_4 absorption edges of three exemplary solids, spanning a broad range of transition energies from a few hundred to several thousands eV. We find that transitions from deep core states, such as the Ti 1*s* states in TiO_2 and the Pb 3*d* states in PbI_2, are ruled by the long-range electron-hole attraction. Spin-orbit coupling and local fields play only a minor role for these excitations, which occur at several keV. The exchange interaction between the excited electron and the core hole becomes more relevant for smaller transition energies, as exemplified with the Ca $L_{2,3}$ edge in CaO. The overlap between Ca 2*p* and 3*d* states calls for a careful treatment of local field effects in order to describe these excitations. Our results, in good agreement with the available experimental data, are thoughtfully analyzed with advanced visualization tools in order to further gain insight into the electronic contributions and the spatial extension of the resulting electron-hole pairs.

TT 18.5 Mon 16:15 GER 38

Non-linear-screening contributions to photoemission spectra — •Marilena Tzavala[1,2], Claudia Rödl[1,2,3], and Lucia Reining[1,2] — [1]Laboratoire des Solides Irradiés, École polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF) — [3]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The state-of-the-art approach to calculate photoemission spectra of a broad range of materials is many-body perturbation theory in the *GW* approximation, sometimes combined with a cumulant expansion. The effective interaction that appears in these approaches is screened within the linear-response approximation. However, the photoemission of a core electron or a localized valence electron may be a strong perturbation, which suggests that non-linear screening effects could be important. We propose a formulation of the functional relations between the one-body Green's function and the screened interaction which is an alternative to Hedin's equations and which explicitly displays non-linear screening. Using a simple model, we show that exchange-correlation contributions are crucial in order to capture the non-linear effects. We also discuss how to apply the scheme to real materials using time-dependent density-functional theory (TDDFT).

TT 18.6 Mon 16:30 GER 38

Dynamic LDA for electronic excitations — •Marco Vanzini[1,2], Matteo Gatti[1,2,3], and Lucia Reining[1,2] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF) — [3]Synchrotron SOLEIL, L'Orme des Merisiers, BP 48 Saint-Aubin, 91192 Gif sur Yvette, France

Density Functional Theory is an extremely useful tool for dealing with ground state properties such as the density or total energy. Kohn–Sham eigenvalues are often considered as approximated electronic excitations, but the resulting spectra are poor.

We propose a generalization of the Kohn–Sham approach to address in an exact framework electron addition and removal spectra. They can be measured by photoemission experiments, and can be evaluated using a computationally expensive non–local Self Energy. Our method is instead based on a frequency–dependent *local* potential [1], which significantly reduces the computing time of an ab–initio calculation.

To find this spectral potential in practice, we propose a jellium–based *dynamical* local density approximation (dynLDA): it relates the unknown potential to its homogeneous counterpart, via a non–trivial connector in space and frequency, which is based on physical insight.

In this talk, I will discuss the achievements and the limits of dynLDA, using models and real solids.

[1] M. Gatti et al., Phys. Rev. Lett. **99**, 057401 (2007).

TT 18.7 Mon 16:45 GER 38

Recent developments of the Sternheimer-GW method — •Martin Schlipf[1], Henry Lambert[1,2], and Feliciano Giustino[1] — [1]Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom — [2]Department of Physics, King's College London, London WC2R 2LS, United Kingdom

The GW many-body perturbation method is an important tool to access accurate band gaps from first principles calculations. The conventional implementation determines the Green's function and the screened Coulomb interaction by a summation over unoccupied states tedious to converge. Giustino et al. demonstrated an alternative method to obtain these quantities by solving Sternheimer linear response equations. In this poster, we present our Sternheimer-GW software implemented in the Quantum Espresso framework and highlight some recent advances regarding the precision and stability of the method. We present our results for a small set of semiconducting materials and compare these to results obtained with conventional GW codes. We illustrate on selected examples the complete frequency dependent self energy, which is a natural product of the Sternheimer-GW method, and can be directly compared to experimental angle-resolved photoemission spectroscopy (ARPES) experiments.

TT 18.8 Mon 17:00 GER 38

Calculating electronic correlations in the CASTEP ab initio code — •Vincent Sacksteder[1] and Evgeny Plekhanov[2] — [1]W155 Wilson Building, Royal Holloway University of London, Egham Hill, Egham, TW20 0EX, — [2]Kings College London

We present new DMFT and GW features in the CASTEP DFT code. These features are designed to provide more accurate treatment of correlations between localized orbitals, of electronic screening, and of excited states. In present benchmarks on Cerium Oxide, the gamma phase of Cerium, and Silicon. We discuss the calculation of atomic forces within the GW framework.

TT 18.9 Mon 17:15 GER 38

Efficient G_0W_0 using localized basis sets: a benchmark for molecules — •Peter Koval[1,2], Mathias Per Ljungberg[1], and Daniel Sánchez Portal[1,2] — [1]Donostia International Physic Center, San Sebastian, Spain — [2]Centro de Fisica de Materiales, San Sebastian, Spain

Electronic structure calculations within Hedin's *GW* approximation are becoming increasingly accessible to the community. In particular, as it has been shown earlier and we confirm by calculations using our **MBPT_LCAO** package [1], the computational cost of the so-called G_0W_0 can be made comparable to the cost of a regular Hartree-Fock calculation. In this work, we study the performance of our new G_0W_0 implementation based on a contour deformation technique to reproduce the ionization potentials of all 117 closed-shell molecules belonging to the G2/97 test set, using a pseudo-potential starting point provided by the popular density-functional package **SIESTA** [2]. Moreover, the ionization potentials and electron affinities of a set of 24 acceptor molecules [3] are compared to experiment and to reference all-electron calculations.

[1] `http://mbpt-domiprod.wikidot.com`; [2] Soler J. M., *etal* J. Phys.: Condens. Matter **14** (2002) 2745; [3] Knight J. W., *etal* J. Chem. Theory Comput., **12** (2016) 615.

TT 18.10 Mon 17:30 GER 38

A dynamic exchange correlation kernel derived from recent results for the homogeneous electron gas — •Martin Panholzer, Matteo Gatti, and Lucia Reining — Laboratoire des Solides Irradies UMR 7642, CNRS-CEA/DSM, Ecole Polytechnique, Palaiseau, France

Time-Dependent Density Functional Theory (TDDFT) is a method of choice to calculate the dynamic structure factor of a wide range of materials. Even in the simplest Adiabatic Local Density Approximation (ALDA), plasmon spectra are generally well described. However, several shortcomings remain. In particular, the onset energy of the spectrum is underestimated [1], and dynamical effects such as lifetime damping and double plasmon excitations are absent [2].

In this work we investigate recent results for the dynamic response of the homogeneous electron gas (HEG)[3] to extract an exchange correlation kernel for TDDFT. In order to get an estimate of the validity of such an approach we compare our results for the dynamic kernel $f_{xc}(q,\omega)$ for the HEG with different kernels and known exact properties. We implemented this kernel with the simplest connection between the HEG and the real material, the mean density approximation. We compare results on simple metals, such as Na and Al, with experiments and ALDA. In order to explore the validity of such an approach we also applied the kernel to Si.

[1] G. Onida et al., Rev. Mod. Phys. 74, 601 (2002)
[2] M. Cazzaniga et al., Phys. Rev. B 84, 075109 (2011)
[3] H. M. Böhm et al., Phys. Rev. B 82, 224505 (2010)

TT 18.11 Mon 17:45 GER 38

Benchmark calculations of the electronic structure for molecules from the second-Born self-energy — •Michael Schüler[1] and Yaroslav Pavlyukh[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany — [2]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, P.O. Box 3049, 67653 Kaiserslautern, Germany

The non-equilbrium Green's function (NEGF) formalism provides a state-of-the-art tool for modeling modern spectroscopic experiments. In particular, time-dependent problems can be treated based on the Kadanoff-Baym equations. The underlying approximation to the self-energy has to be consistent with the treatment of the initial state - as captured by the Matsubara formalism - in order to guarentee the basic conservation laws. One of simplest non-trivial approximation to the self-energy is the second-Born approximation (2BA), which has been employed in numerous time-dependent studies. Systematic tests on the accuracy of the 2BA for various molecules has, however, been lacking so far. In our contribution we fill this gap by benchmark calculations for the 2BA for small molecules from the well established G2 test set. We demonstrate that the accuracy of the 2BA for predicting ionization potentials and electron affinities can compete with accurate quantum chemistry methods such as the Møller-Plesset perturbation theory and the coupled-cluster method. We also apply our method to a class of larger molecules, the diamonoids, which are in the focus of recent experiments and theoretical studies.

TT 18.12 Mon 18:00 GER 38

Performance of the GW approximation at reproducing key features in exact Kohn-Sham potentials — •Jack Wetherell[1], Leopold Talirz[1], Matt Hodgson[2], and Rex Godby[1] — [1]University of York, York, United Kingdom — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

One of the major goals of the GW method is to improve the accuracy of charge densities produced by density functional theory (DFT). In this work we test the applicability of one-shot GW from various DFT starting Kohn-Sham orbitals. Also we implement and test the fully self-consistent GW method. We test the applicability of these methods by using them to compute densities for simple model 1D systems from which the exact density can be obtained by the direct solution of the Schrodinger Equation. We choose a set of test systems that are either dominated by exchange or correlation, or contain non-local steps in the exact exchange-correlation potential. Also we analyse systems dominated by electronic interaction. We can also investigate how accurate the exchange-correlation potentials associated with the GW densities are, using our reverse-engineering algorithm.

TT 19: Poster Session: Correlated Electrons 1

Time: Monday 15:00–19:00 Location: P2-EG

TT 19.1 Mon 15:00 P2-EG

Bulk and surface properties of $SmRh_2Si_2$ single crystals — •Jacintha Banda[1], Kristin Kliemt[2], Alla Chikina[3], Alexander Generalov[4], Kurt Kummer[5], Monika Güttler[3], Victor N. Antonov[6], Yuri Kucherenko[6], Steffen Danzenbächer[3], Christoph Geibel[1], Clemens Laubschat[3], Denis V. Vyalikh[3,7,8,9], Cornelius Krellner[2], and Manuel Brando[1] — [1]MPI CPfS, Dresden, Germany — [2]Goethe-University Frankfurt, Frankfurt, Germany — [3]Dresden University of Technology, Dresden, Germany — [4]MAX IV Laboratory, Lund, Sweden — [5]ESRF, Grenoble, France — [6]National Academy of Sciences of Ukraine, Kiev, Ukraine — [7]Saint Petersburg State University, Saint Petersburg, Russia — [8]Donostia International Physics Center, San Sebastian, Spain — [9]IKERBASQUE, Bilbao, Spain

We present the properties of $SmRh_2Si_2$. Using a modified Bridgman method with indium flux we obtained platelet-shaped $SmRh_2Si_2$ single crystals. The magnetic ground state was characterized by magnetization, specific heat and electrical transport measurements. $SmRh_2Si_2$ orders antiferromagnetically below $T_N = 62\,K$ with pronounced anomalies in C(T) and ρ(T). Due to the layered structure, the crystals could be cleaved easily parallel to the Sm-layers leading to well-defined atomically flat surfaces allowing to perform ARPES to investigate the valence of the Sm ions in the bulk and at the surface [1]. We found that, in spite of the antiferromagnetic order, Sm reveals divalent admixtures to the almost trivalent ground state both in the bulk and at the surface. [1] A. Chikina et al., to be published

TT 19.2 Mon 15:00 P2-EG

An Ultrasonic Study of the Heavy-Fermion Metal $YbNi_4P_2$ — •Yeekin Tsui, Lars Postulka, Bernd Wolf, Ulrich Tutsch, Kristin Klimt, Cornelius Krellner, and Michael Lang — Goethe-Universität, Physikalisches Institut SFB/TR49, D-60438 Frankfurt(M), Germany

$YbNi_4P_2$ is a stoichiometric heavy-fermion Kondo-lattice system with a Kondo temperature TK $\sim$ 8 K. The material exhibits unique features among the heavy-fermion compounds including its quasi-1D crystalline and electronic structure. Furthermore, $YbNi_4P_2$ undergoes a second-order ferromagnetic (FM) phase transition at 0.17 K, which can be suppressed by doping with a small amount of As leading to a FM quantum-critical point (QCP). The 4f-spins remain strongly fluctuating down to the lowest measured temperatures which influence the thermodynamic and transport properties of $YbNi_4P_2$. Therefore, $YbNi_4P_2$ is the first clean system situated in the close vicinity of an FM QCP [1]. Ultrasonic measurements have proven to be a powerful probe for characterizing the intriguing properties of heavy-fermion metals. Here we present ultrasonic measurements on a single crystal of $YbNi_4P_2$ over a wide temperature range. Our data show clear features in the ultrasound velocity and the attenuation corresponding to crystal-electric-field effects around 30 K. Further ultrasonic measurements are being conducted at temperatures around the FM phase transition.

[1] C. Krellner et al., New Journal of Physics 13 (2011) 103014

TT 19.3 Mon 15:00 P2-EG

Low Energy Dynamics in Charge Ordered $R_{0.5}Sr_{0.5}MnO_3$ (R = Nd and Pr) Manganite Thin Films — •Rakesh Rana[1], Johannes Schmidt[1,2], Jorg Grenzer[1], Harald Schneider[1], Manfred Helm[1,2], and Alexej Pashkin[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

The half-doped $Pr_{0.5}Sr_{0.5}MnO_3$ manganite represents a unique stripe type CO-orbital order that induces transport and magnetic anisotropy whereas the CO in $Nd_{0.5}Sr_{0.5}MnO_3$ is charge-exchange (CE)-type which is isotropic in nature.

We have systematically explored epitaxial manganite thin films grown on (100), (110), and (111) oriented $(LaAlO_3)_{0.3}(Sr_2TaAlO_6)_{0.7}$ substrates by pulsed laser deposition technique. Our Terahertz time-domain spectroscopic data reveal charge density wave (CDW) resonance centered around 5-6 meV for (110) oriented films and Drude-like conductivity for (100) and (111) oriented films. The CDW resonance in the optical conductivity spectra can be tuned from 4 meV to 6 meV for (110) oriented films and depends on the amount of ferromagnetic phase fraction in the CO matrix and corroborates well with the magnetization measurements. The nonlinear conductivity related to the sliding of the pinned CDW character makes the studied systems promising candidates for ultrafast coherent control of charge transport by resonant THz pumping.

TT 19.4 Mon 15:00 P2-EG

DFT simulations of rare-earth hexaborides using hybrid functionals — •Florian Sohn[1] and Peter Blöchl[1,2] — [1]Institut für theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institut für theoretische Physik, Technische Universität Clausthal, Leibnizstr. 10, 38678 Clausthal-Zellerfeld

Rare-earth hexaborides (REB_6) are strongly correlated materials, where the strong Coulomb interaction between electrons in the rare-earth's f-electron shell influence the electronic properties of the whole material decisively.

Rare-earth hexaborides exhibit a variety of low-temperature phenomena, including antiferromagnetic ordering for most partially filled f-shells, ferromagnetic ordering in EuB_6, superconductivity in LuB_6, topological insulating behavior in SmB_6 and a complex phase diagram with Kondo behavior in CeB_6. We present results of density functional theory calculations using the local hybrid functional PBE0. The hybrid functional accounts for some of the more important correlations and thus provides a viable starting point for many-particle calculations using more sophisticated many-particle methods. The calculations are done with the PAW method using our CP-PAW code, which describes the f-electrons explicitly. The electronic structure is rationalized on the basis of the projected density of the systems and their changes throughout the series.

We gratefully acknowledge financial support by the DPG project PR298/19-1.

TT 19.5 Mon 15:00 P2-EG

Coupling of Co atoms on Cu(111) through monatomic chains — •Neda Noei, Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel

Using a low temperature scanning tunneling microscope we investigated how the Kondo resonance of a single Co atom on Cu(111) changes when it is attached to monatomic Cu chains. Cu chains with lengths up to 100 nm were repeatedly fabricated. They are one type of dislocations which arise after dipping the tip into Cu(111). In order to evaluate a long range interaction between magnetic atoms, Co atoms were attached to the copper chains at different distances from each other. We observed a nonuniform variation of the Kondo resonance in amplitude and width.

TT 19.6 Mon 15:00 P2-EG

Realistic description of multi-orbital Kondo Anderson impurities on metal surfaces — •Francisco Meirinhos, Ammar Nejati, and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

The detailed understanding of the STM spectra of magnetic atoms adsorbed on a metal surface is hampered by the complexity of the atomic level scheme consisting of multiple local orbitals, occupied by several electrons. We develop a quantitative theory for the description of such complex Anderson impurities which proceeds in three steps. (1) We transform the atomic multi-orbital, multi-electron states to the local eigenstate basis, involving Hund's rules and the Clebsch-Gordan coefficients, in order to determine the multiplet of low-lying spin-orbit Kramers doublets of the magnetic atom. Taking into account local charge fluctuations by at most one unit, this defines an effective multi-orbital, infinte$-U$ Anderson impurity model. (2) The parameters of this model are determined by fitting the (magnetically polarized) spectra of the mean-field solution to the results of spin-polarized density functional theory (DFT). This is accurate for the high-energy spectral features. (3) Finally, we calculate the low-energy Kondo-Fano spectra for the obtained parameters using the multi-orbital non-crossing approximation (NCA). The results will be compared with experimental STM dI/dV spectra.

TT 19.7 Mon 15:00 P2-EG

Ward identities versus two-particle self-consistency — •Friedrich Krien[1], Erik G.C.P. van Loon[2], Hartmut Hafermann[3], Alexander I. Lichtenstein[1], and Mikhail I. Katsnelson[2] — [1]Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Radboud University, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands — [3]Mathematical and Algorithmic Sciences Lab, France Research Center, Huawei Technologies Co. Ltd., 92100 Boulogne Billancourt, France

Some diagrammatic extensions of (E)DMFT (EDMFT+GW, Trilex, Dual Boson and others) introduce retarded interactions into the Anderson-Impurity model to fix a two-particle self-consistency condition. We take a close look at the fate of conservation laws under this pretext and demonstrate that Φ-derivability à la Baym-Kadanoff is not a sufficient criterion for spin conservation. We propose direct numerical validation to verify Ward identities.

TT 19.8 Mon 15:00 P2-EG

Electron spin resonance as a function of frequency, field, temperature, and angle using broadband and resonant planar microwave devices applied to $YbRh_2Si_2$ and ruby — •Linda Bondorf[1], Manfred Beutel[1], Wolfgang Voesch[1], Markus Thiemann[1], Kristin Kliemt[2], Cornelius Krellner[2], Martin Dressel[1], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Goethe-Universität, Frankfurt am Main, Germany

The quantum-critical heavy-fermion material $YbRh_2Si_2$ shows strong magnetic anisotropy and exhibits antiferromagnetic order at temperatures below 70 mK and magnetic fields below 60 mT. Electron spin resonance (ESR) measurements on $YbRh_2Si_2$ at such low temperatures and fields are highly desired but out of reach for conventional ESR spectrometers. These limitations can be overcome with resonant and broadband planar microwave devices as ESR probes [1, 2].

Here we present an ESR setup that enables frequency-, magnetic field-, temperature-, and angle-dependent measurements using coplanar structures. We demonstrate this technique through broadband ESR measurements (up to 20 GHz) on ruby with in-situ sample rotation inside a ^{4}He cryostat. Angle-dependent measurements with enhanced sensitivity on $YbRh_2Si_2$ are performed down to 4.4 GHz and 1.6 K using a superconducting coplanar resonator, and extensions of this approach to mK temperatures will be discussed.

[1] M. Scheffler *et al.*, Phys. Status Solidi B **250**, 439 (2013).
[2] Y. Wiemann *et al.*, Appl. Phys. Lett. **106**, 193505 (2015).

TT 19.9 Mon 15:00 P2-EG

Characterization of As substituted $YbNi_4P_2$ single crystals — •Philipp Ross, Kristin Kliemt, and Cornelius Krellner — Institute of Physics, Goethe-University Frankfurt, D-60438 Frankfurt, Germany

The tetragonal compound $YbNi_4P_2$ has a low Curie temperature, T_C = 0.17 K, which can be further suppressed by substituting P by As. The rare case of a ferromagnetic quantum critical point occurs in the substitution series $YbNi_4(P_{1-x}As_x)_2$ at x≈0.1 [1,2].

Single crystals of $YbNi_4(P_{1-x}As_x)_2$, with various As concentrations were grown by the Czochralski method [3]. Strong effort was undertaken to determine the precise orientation of the as-grown crystals and prepare single-crystalline pieces. These crystals were characterized by electrical transport, heat capacity and magnetization measurements. Here we present the measured data these measurements down to T = 2 K. Furthermore, we characterized the room temperature crystal structure by powder X-ray diffraction and determined the change in the lattice constants for increasing As content using Rietveld refinement.

[1] C. Krellner et al., New J. Phys. 13, 103014 (2011)
[2] A. Steppke et al., Science 339, 933 (2013)
[3] K. Kliemt, C. Krellner, J. Cryst. Growth 449, 129-133 (2016)

TT 19.10 Mon 15:00 P2-EG

Magnetic anisotropy in $YbNi_4P_2$ — •Sven Friedemann[1], Sara Karbassi[1], Saman Ghannadzadeh[2], Manuel Brando[3], Kristin Kliemt[4], and Cornelius Krellner[4] — [1]HH Wills Laboratory, University of Bristol, UK — [2]High Field Magnet Laboratory, University of Radboud, Nijmegen, NL — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Frankfurt am Main, Germany

$YbNi_4P_2$ is a rare example of a heavy-fermion compound with ferromagnetic (FM) order. It allows to study the emergence of a FM quantum critical point (QCP) which marks a long-standing challenge in metallic compounds as FM QCPs are avoided in most systems through a change of the transition to 1st order or through an intervening antiferromagnetic phase. $YbNi_4P_2$ by contrast was demonstrated to have a readily accessible QCP when suppressing the FM order with substitution of phosphorous by arsenic [1]. An alternative route to access the FM QCP could be via a transverse field tuning for strongly anisotropic FM order. We use angular dependent magnetoresistance measurements to extract the anisotropy of the Landé g factor. This will be the basis to understand under which conditions a FM QCP may be accessed via transverse field tuning.

[1] Steppke, A., et al., Science, **339**, 933 (2013).

TT 19.11 Mon 15:00 P2-EG

Evolution of the entropy in the magnetic phases of partially frustrated CePdAl — •Kai Grube[1], Stefan Lucas[2], Chien-Lung Huang[1,2,3], Akito Sakai[4], Sarah Woitschach[2], Elizabeth L. Green[5], Sebastian Kuntz[1], J. Wosnitza[5], Veronika Fritsch[4], Philipp Gegenwart[4], Oliver Stockert[2], and Hilbert von Löhneysen[1,3] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [3]Physikalisches Institut, Karlsruher Institut für Technologie, Germany — [4]Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, Germany — [5]Hochfeld-Magnetlabor Dresden (EMFL-HLD), Helmholtz-Zentrum Dresden-Rossendorf, Germany

In the heavy-fermion metal CePdAl long-range antiferromagnetic order coexists with geometric frustration of one third of the Ce moments. At low temperatures the Kondo effect tends to screen the frustrated moments. We use magnetic fields B to suppress the Kondo screening and studied the magnetic phase diagram and the evolution of the entropy with B employing thermodynamic probes. We estimate the frustration by introducing a definition of the frustration parameter based on the enhanced entropy, a fundamental feature of frustrated systems. In the field range where the Kondo screening is suppressed the liberated moments tend to destabilize the magnetic order and strongly enhance the frustration.

TT 19.12 Mon 15:00 P2-EG

Magnetic correlations in Ce(Pt,Pd)Al_3 — •Stefan Weber[1], Petr Cermak[2], Christian Franz[1], Wolfgang Simeth[1], Kirill Nemkovskiy[2], Astrid Schneidewind[2], and Christian Pfleiderer[1] — [1]Physik-Department, Technische Universität München, Garching, DE — [2]Jülich Centre for Neutron Science, MLZ, Garching, DE

The nature of quantum phase transitions in selected Ce compounds is still heavily discussed [1]. The properties of these systems are characterized by the interplay of several competing energy scales. In the Ce$T$$Al_3$ (T=transition metal) series, T=Pt and Pd compounds are located at the border of antiferromagnetic ordering but not known to order yet [2]. Extensive measurements of the bulk properties (magnetization, susceptibility and specific heat) suggest the possible collapse of energy scales across the quantum phase transition in these systems [3]).

We studied single crystals of $CePtAl_3$ and $CePdAl_3$ by polarized neutron diffraction on DNS (MLZ Garching) at very low temperatures. A search for long-range magnetic order in $CePtAl_3$ appears to be inconclusive so far with putative evidence for magnetic reflections and hysteresis. In contrast, in $CePdAl_3$ we find clear evidence for magnetic order at low temperatures. The possible magnetic structures of both compounds will be discussed.

[1] P. Gegenwart, Q. Si, F. Steglich e.g. Nature Physics 4, 186 (2008).
[2] C. Franz, et al., J. Alloys Compd. 688, 978 (2016)
[3] C. Franz, PhD thesis, TU Munich (2014)

TT 19.13 Mon 15:00 P2-EG

Advancing the crystal quality and dimensions in the crystal growth process of $Yb(Rh_{1-x}Ir_x)_2Si_2$ — •Sebastian Witt[1], Michael Baenitz[2], and Cornelius Krellner[1] — [1]Goethe University Frankfurt, 60438 Frankfurt am Main, Germany — [2]MPI for Chemical Physics of Solids, 01187 Dresden, Germany

In the heavy fermion compound, $YbRh_2Si_2$, a superconducting phase transition at 2mK was found recently [1]. From these measurements it is further evident, that the occurence of nuclear antiferromagnetic order slightly above T_C plays an essential role. Single crystals (SC) with isotope pure silicon and/or ytterbium enable the investigation of the nature of the superconductivity in this material. Additionaly, the

stability of the superconduction phase can be investigate by the substitution of rhodium by iridium. Due to small amounts of the isotopes and the non-nominal and non-homogenous substitution it is necessary to further optimize the crystal growth.

Here, we report the crystal growth of $Yb(Rh_{1-x}Ir_x)_2Si_2$ with the optimized accelerated crucible rotation technique. This technique enhances the crystal quality (homogeneity, less distortions and reduced flux inclusions). The process optimization is accompanied by resistivity measurements of the SCs as well as EDX measurements to ensure the homogeneity of the substituted elements. We report simulations of the growth process inside the crucible. Crystals with the silicon-29 isotope were used for first NMR measurements and results of metallothermic reduction of Yb_2O_3 to obtain the Yb-metal were presented.

[1] E. Schuberth et al., Science, **351(6272)**, 485-488, (2016).

TT 19.14 Mon 15:00 P2-EG

Novel Quantum Criticality in the Au-Al-Yb Quasicrystal — •Andreas Wörl[1], Shuya Matsukawa[2], Akito Sakai[3], Noriaki Sato[2], and Philipp Gegenwart[1] — [1]Experimentalphysics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Department of Physics, Graduate School of Science, Nagoya University, Japan — [3]Institute for Solid State Physics, The University of Tokyo, Japan

The emergence of non-Fermi liquid behavior without tuning an external control parameter has been reported for several heavy-fermion materials lately. One prime example is the icosahedral quasicrystal $Au_{51}Al_{36}Yb_{15}$, which exhibits divergent behavior of magnetic susceptibility, $\chi^{-1} \propto T^{0.51}$, and specific heat, $C/T \propto -\ln T$, in zero magnetic field [1].

To further resolve the nature of the non-Fermi liquid state, we report thermal expansion and magnetostriction measurements at ultra-low temperatures. The Grüneisen ratio, which is the most suitable physical quantity for the characterization of pressure sensitive quantum crititcal phenomena, gives no evidence of an intrinsically generated pressure sensitive quantum critical point. We conclude the formation of a novel critical state with the peculiarity of low pressure but high magnetic field sensitivity.

[1] K. Deguchi, S. Matsukawa, N. K. Sato, T. Hattori, K. Ishida, H. Takakura and T. Ishimasa, Nat. Mater. **11**, 1013 – 1016 (2012)

TT 19.15 Mon 15:00 P2-EG

Thermal expansion measurements on $Cs_2CuCl_{4-x}Br_x$ at sub-Kelvin temperatures — •Satya Krishna Thallapaka, Christian Thurn, Ulrich Tutsch, Bernd Wolf, and Michael Lang — Physikalisches Institut, SFB/TR49, Goethe Uni Frankfurt, DE

In recent years, Cs_2CuCl_4 and Cs_2CuBr_4 have been extensively investigated both experimentally and theoretically, as they represent model systems for quasi-2D triangular-lattice quantum antiferromagnets. They attracted much attention due to their unconventional magnetic properties resulting from the interplay of strong quantum fluctuations in reduced dimensions, geometrical frustration and effects of spin-lattice interactions close to the field-induced quantum critical point (QCP). Recently, a study of the mixed system $Cs_2CuCl_{4-x}Br_x$ has identified two novel compounds [1] with well-ordered halide sublattices due to a site-selective substitution mechansim, namely $Cs_2CuCl_3Br_1$ and $Cs_2CuCl_2Br_2$. It was predicted that the latter compound is showing an even higher degree of frustration than the border compounds. Thus, the series $Cs_2CuCl_{4-x}Br_x$ is ideal to study the effects of frustration and dimensionality around the QCP. To this end, we will present measurements of the thermal expansion coefficient on Cs_2CuCl_4 down to $T = 40$ mK around the field-induced QCP. The thermal expansion coefficient has been proven to be particularly suited to probe the anomalous thermodynamics of QCPs [2]. In addition, we will compare these results to measurements of the thermal expansion on the mixed system $Cs_2CuCl_2Br_2$ and to specific heat measurements.

[1] Cong *et al.*, PRB **83**, 064425 (11)
[2] Zhu *et al.*, PRL 91, 066404 (03)

TT 19.16 Mon 15:00 P2-EG

Spin dynamics of $FeGa_{3-x}Ge_x$ studied by Electron Spin Resonance — Bonho Koo[1], Kristian Bader[2], Michael Baenitz[1], Peter Gille[2], and •Jörg Sichelschmidt[1] — [1]MPI für Chemische Physik fester Stoffe, Dresden — [2]LMU, Kristallographie, München

$FeGa_3$ is a nonmagnetic, narrow-gap semiconductor which acquires itinerant ferromagnetism upon electron doping by a partial replacement of Ga with Ge. The way how this magnetism evolves is of particular interest for better understanding the *d*-electron heavy-fermion behaviour of $FeGa_{3-x}Ge_x$ (at $x < 0.15$) or the properties close to a ferromagnetic (FM) quantum critical point at the critical Ge-concentration of $x = 0.15$. For detailed studies in this direction the availability of single crystals with a high purity is a precondition.

We studied the electron spin resonance (ESR) of ultra-pure single crystals of $FeGa_{3-x}Ge_x$ for $x = 0$ and x around 0.15. For $x = 0$ we observed a well-defined ESR signal, indicating the presence of pre-formed magnetic moments in the semiconducting phase. Upon increasing x the occurrence of itinerant magnetism clearly affects the ESR properties below $T \approx 30$ K whereas at higher T an ESR signal as seen in $FeGa_3$ prevails independent on the Ge-content. We interpret the low-T ESR in terms of a resonance of conduction electron spins and consider the relaxation as being determined by exchange fields. This is supported by a comparison with the temperature dependencies of magnetisation and electrical resistivity. The present results show that the ESR of $FeGa_{3-x}Ge_x$ is an appropriate and direct tool to investigate FM correlations in the vicinity of a FM quantum critical point.

TT 19.17 Mon 15:00 P2-EG

Quantum Monte Carlo simulations of metallic quantum critical points — •Carsten Bauer[1], Yoni Schattner[2], Erez Berg[2], and Simon Trebst[1] — [1]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [2]Department of Condensed Matter Physics, The Weizmann Institute of Science, Rehovot, 76100, Israel

While quantum critical phenomena in insulators are relatively well understood, their metallic counterparts pose a substantial theoretical challenge since the order parameter fluctuations can interact with gapless fermionic excitations on the Fermi surface. This interplay, however, allows for a multitude of competing orders in the vicinity of a metallic quantum critical point including e.g. the formation of superconductivity when driving the metallic system through a phase transition.

Fortunately, it has recently been demonstrated that for certain classes of metallic quantum critical points this physics can be studied by determinant quantum Monte Carlo simulations, without suffering from the notorious fermion "sign problem". I will show numerically exact studies of the antiferromagnetic quantum critical point in two spatial dimensions and discuss techniques to improve on the scalability of the determinant quantum Monte Carlo approach.

TT 19.18 Mon 15:00 P2-EG

Phase diagram of the quantum dissipative rotor model with two competing baths — •Dominik Maile[1], Sabine Andergassen[1], Wolfgang Belzig[2], and Gianluca Rastelli[2] — [1]Eberhard Karls Universität Tübingen, D-72074 Tübingen, Germany — [2]Universität Konstanz, D-78457 Konstanz, Germany

We study a quantum dissipative rotor model in which each local phase-difference and each local momentum are uniformly coupled to two different baths. Such systems can represent e.g. a chain of resistively shunted Josephson junctions [1], capacitively coupled to a diffusive metal [2]. The first dissipative coupling quenches the quantum phase fluctuations favoring the long-range phase order (i.e. superconducting ground state) whereas the second one quenches momentum fluctuations destroying phase coherence (insulating ground state).

Using the Self-Consistent Harmonic Approximation [1], we calculate the zero-temperature phase diagram as determined by the two dissipative coupling constants and the bare zero point fluctuations. As an effect of the quantum frustration for the two canonical conjugate observables [3], we obtain an interesting phase diagram with a non-monotonic behavior: for instance, the ground state can pass from superconducting to insulating phase and back to superconducting phase by increasing the dissipation.

[1] S. Chakravarty et al., Phys. Rev. Lett. **56**, 2303 (1986).
[2] A.M.Lobos, T. Giamarchi, Phys. Rev. B **84**, 024523 (2011).
[3] G. Rastelli, New J. Phys. **18**, 053033 (2016).

TT 19.19 Mon 15:00 P2-EG

Competing phases in spin ladders with ring exchange and frustration — •Alexandros Metavitsiadis[1] and Sebastian Eggert[2] — [1]Institute for Theoretical Physics Technical University Braunschweig, Braunschweig, Germany — [2]Department of Physics and OPTIMAS Research Center, University of Kaiserslautern, Kaiserslautern, Germany

The ground state properties of spin-1/2 ladders are studied, emphasizing the role of frustration and ring exchange coupling. We present a unified field theory for ladders with general coupling constants and

geometry. Rich phase diagrams can be deduced by using a renormalization group calculation for ladders with in chain next nearest neighbor interactions and plaquette ring exchange coupling. In addition to established phases such as Haldane, rung singlet, and dimerized phases, we also observe a surprising instability towards an incommensurate phase for weak interchain couplings, which is characterized by an exotic coexistence of self-consistent ferromagnetic and anti-ferromagnetic order parameters.

TT 19.20 Mon 15:00 P2-EG

Magnetic phase diagram of $LuFe_4Ge_2$ under high pressure probed by μSR — •Shanu Dengre[1], Rajib Sarkar[1], M.O. Ajeesh[2], Philipp Materne[1], Rustem Khasanov[3], Katharina Weber[2], Christoph Geibel[2], Michael Nicklas[2], and Hans-Henning Klauss[1] — [1]Institute for Solid State Physics, TU-Dresden, 01069-Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187-Dresden, Germany — [3]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, CH-5232-Villigen, Switzerland

$LuFe_4Ge_2$ is a geometrically frustrated magnetic system with antiferromagnetic (AFM) ordering at $T_N = 36$ K. In this work, we used μSR spectroscopy to study the pressure evolution of magnetic phase diagram of $LuFe_4Ge_2$. Previous electrical transport investigations showed a continuous suppression of T_N to zero temperature at 1.7 GPa and suggested the existence of a second pressure-induced magnetic phase. Our transverse field - μSR experiments find a 100% magnetic volume below T_N in the low pressure AFM phase. Further, they prove the presence of a second long-range antiferromagnetically ordered phase at higher pressures and also indicate that the complete sample volume is magnetically ordered in this phase. The obtained ordering temperatures are in good agreement with the electrical resistivity data. The low temperature muon precision frequency does not change between zero and 2.25 GPa, which is consistent with a similar size of the ordered moment in the two different magnetic phases.

TT 19.21 Mon 15:00 P2-EG

Magnetic order and spin dynamics in a helical magnetic system $Fe_3PO_4O_3$ — •Rajib Sarkar[1], Sirko Kamusella[1], Sascha Albert Bräuninger[1], Stefan Holenstein[2], Hubertus Luetkens[2], James Neilson[3], Michael Tarne[3], Kate Ross[3], and Hans-Henning Klauss[1] — [1]Institute for Solid State Physics, TU Dresden, D-01069, Germany — [2]Department of Physics, Colorado State University, Fort Collins, Colorado 80523-1875, USA — [3]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen, Switzerland

The 3d-electronic spin dynamics and the magnetic order in $Fe_3PO_4O_3$ were investigated by μSR and the ^{57}Fe Mössbauer experiments. Zero field (ZF)-μSR and the ^{57}Fe Mössbauer studies prove the static long range magnetic ordering below $T_N \approx 163$ K. Both transverse field (TF) and ZF-μSR results evidence 100% magnetic volume fraction in the ordered state. ZF-μSR time spectra can be best described by a Bessel function which is consistent with the helical type of magnetic structure as proposed by the neutron scattering experiments. ^{57}Fe Mössbauer results are also consistent with the helical magnetic structure. While spin-lattice relaxation rate (λ) exhibits a peak at the magnetic ordering related to the critical fluctuations, another peak shows up also at around 35 K signaling the presence of secondary relevant energy scale in $Fe_3PO_4O_3$.

TT 19.22 Mon 15:00 P2-EG

Magnetic order and spin dynamics in $La_2O_2Fe_2O(S/Se)_2$ probed by ^{57}Fe Mössbauer and ^{139}La NMR spectroscopy — •Sirko Kamusella[1], Rajib Sarkar[1], Felix Brückner[1], Vadim Grinenko[1], Hans-Henning Klauss[1], and Byron Freelon[2] — [1]Institute for Solid State Physics, TU Dresden, D-01069, Germany — [2]Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139, USA

We present ^{57}Fe Mössbauer and ^{139}La NMR studies on $La_2O_2Fe_2OS_2$ in the magnetically ordered state and paramagnetic state. Similar to $La_2O_2Fe_2OSe_2$ [1] we observed a non collinear magnetic structure in $La_2O_2Fe_2OS_2$, accounting for the explicitly broken x-y-symmetry in the layered structure. The magnetism in this compound is based on frustrated J1-J1'-J2 interactions and single-ion anisotropy. However, unexpected observations occurred: The continuous reduction of the principal component V_{zz} of the EFG below $1.4T_N$ for both compounds and the continuous slowing down of the spin fluctuations as reflected in the NMR spin lattice relaxation rate ($^{139}T_1$) could be discussed in the context of spin-nematicity.

Therefore, parts of our investigations can be related to advanced theoretical concepts which are used to model the physics in these materials, such as orbital selective Mottness [2], biquadratic spin interactions and two magnon relaxation.

[1] M. Günther *et al.*, Phys. Rev. B. **90** 184408 (2014)
[2] L. Craco *et al.*, J. Phys. Condens Matter. **26**, 145602 (2014)

TT 19.23 Mon 15:00 P2-EG

Persistent spin dynamics in $NaCaCo_2F_7$ as evidenced by μSR — •Sascha Albert Bräuninger[1], Rajib Sarkar[1], Jason W. Krizan[2], Shanu Dengre[1], Philip Materne[1], Chris Baines[3], Hubertus Luetkens[3], Robert J. Cava[2], and Hans-Henning Klauss[1] — [1]Institute for Solid State Physics, TU Dresden, D-01069, Germany — [2]Department of Chemistry, Princeton University, Princeton, NJ 08544, USA — [3]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen, Switzerland

The fluoride pyrochlore $NaCaCo_2F_7$ is a newly discovered frustrated pyrochlore with a frustration index of $f = \frac{|\theta_{CW}|}{T_f} \approx 56$. While recent NMR experiments on $NaCaCo_2F_7$ suggested a spin frozen state below 3 K, neutron scattering experiments on the other hand proposed XY like antiferromagnetic spin clusters at low energies. We present μSR studies on $NaCaCo_2F_7$. Present results indicate the slowing down of the magnetic spin fluctuation upon cooling towards the NMR and neutron scattering spin frozen state transition temperature of $T_{sf} \approx 3.0$ K. The μSR relaxation rate increases slightly below this frozen state, and remains constant down to 20 mK. In the μSR window there is no indication of static magnetism in $NaCaCo_2F_7$. In longitudinal field (100-4000 G) the relaxation rate do not vary indicating that the spin fluctuations are dynamic, and this is persistent even at $T \approx 20$ mK. While persistent spin dynamics (PSD) appears to be a generic feature of frustrated magnetic systems, it is not clear so far for the present case whether this is associated with quantum fluctuations, spin-liquid physics, or some other effect.

TT 19.24 Mon 15:00 P2-EG

Magnetostriction and Thermal Expansion of α-$RuCl_3$ — •Mohammad Hossein Haghighi[1], Laura T. C. Bohórquez[1], Anja U. B. Wolter[1], Paula J. Kelley[3,4], Stephen E. Nagler[4], and Bernd Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01062 Dresden, Germany — [3]Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee 37996, USA — [4]Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

α-$RuCl_3$ crystallizes in a layered honeycomb structure and has been proposed as a candidate to realize a fractionalized Kitaev model with strongly frustrated, bond-dependent, anisotropic interactions between Ru^{3+} magnetic moments. We report on angular dependent dilatometric measurements of α-$RuCl_3$, probing the thermal expansion of its lattice as well as its coupling to the magnetic spins via magnetostriction experiments in a wide range of temperatures and magnetic fields. By combining the changes of the thermal expansion and the heat capacity at the magnetic transition via the Ehrenfest relation, strong and anisotropic uniaxial pressure dependencies of α-$RuCl_3$ have been revealed.

TT 19.25 Mon 15:00 P2-EG

High-field ESR studies of the strong-leg spin-1/2 ladder antiferromagnet DIMPY — •A.N. Ponomaryov[1], J. Wosnitza[1,2], K. Povarov[3], D. Schmidiger[3], A. Zheludev[1], and S.A. Zvyagin[1] — [1]Hochfeld-magnet Labor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Dresden, Germany — [3]Neutron Scattering and Magnetism, Laboratory for Solid State Physics, ETH Zürich, Switzerland

We report on high-field ESR studies of the Cu^{2+}-based strong-leg spin-1/2 ladder antiferromagnet $(C_7H_{10}N)_2CuBr_4$ (also known as DIMPY). ESR spectra were measured at frequencies from 58 to 450 GHz at 1.5 K. In addition to the gapped mode observed previously [M. Ozerov et al., Phys. Rev. B **92**, 241113(R) (2015)] a fine structure of the gapless mode was revealed. The data were analyzed employing ESR exchange narrowing theory, allowing us to estimate the interladder exchange interaction, $J' = 77$ mK. Further peculiarities of the ESR spectra of

DIMPY will be discussed.

This work was partly supported by the DFG.

TT 19.26 Mon 15:00 P2-EG

Low temperature thermodynamic properties of the quantum spin liquid candidate $YbMgGaO_4$ — •Sebastian Bachus, Yoshifumi Tokiwa, Andreas Wörl, Yuesheng Li, and Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

A quantum spin liquid (QSL) is a new state of matter which shows no ordering of its magnetic moments even at lowest temperatures. It has attracted a lot of attention in the last years due to its exotic behaviour as well its relevance for high temperature superconductors [1].
Recently, the very promising QSL candidate $YbMgGaO_4$ has been found, where the Yb^{3+}-ions form a triangular lattice. Heat capacity and Muon spin relaxation measurements down to 0.05 K provide evidence for the formation of a U(1) QSL ground state [2-4].
Since the antiferromagnetic coupling constant J is in the order of 1 K, further investigations of the low temperature properties are crucial for a better understanding of this compound.
Here, we report various low temperature measurements of specific heat, thermal expansion and magnetostriction down to 40 mK.

[1] P. A. Lee, Rep. Prog. Phys., **71** (2008)
[2] Y. Li et al., Sci. Rep., **5**, 16419 (2015)
[3] Y. Li et al., Phys. Rev. Lett., **115**, 167203 (2015)
[4] Y. Li et al., Phys. Rev. Lett., **117**, 097201 (2016)

TT 19.27 Mon 15:00 P2-EG

Characterization and optimized synthesis parameters of haydeeite α-$Cu_3Mg(OH)_6Cl_2$, an S = 1/2 kagome magnet — •Joy Desor, Pascal Puphal, and Cornelius Krellner — Physikalisches Institut, Goethe-University Frankfurt, 60438 Frankfurt am Main, Germany

Haydeeite α-$Cu_3Mg(OH)_6Cl_2$ is one of the few examples of $S = \frac{1}{2}$ kagome magnets, that do not show the conventional Néel order at low temperatures[1]. It is the Mg equivalent of kapellasite, the isostructural compound of the prominent spin liquid candidate herbertsmithite.

We present the results of the haydeeite synthesis via the known reflux and a new hydrothermal approach. We have varied several parameters, as e.g. molar ratios, time and temperature gradient. The results were analyzed by PXRD and EDS. This will serve as a starting point for the crystal growth under hydrothermal conditions. Observation of the magnetic properties at low temperatures and specific heat reveals the features of highly frustrated kagome systems.

[1] R.H. Colman, A. Sinclair, and A.S. Wills, Chem. Mat. 22, 5774 (2010).

TT 19.28 Mon 15:00 P2-EG

New 3d-5d double perovskites containing Ir^{5+} — •Klaus K. Wolff[1], Martin Jansen[2], Alexander C. Komarek[1], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

Double perovskites with the general formula $A_2BB'O_6$ (A = alkaline-earth or rare earth metal, B = 3d transition metal, B' = 4d or 5d transition metal) with an ordered rock-salt-like arrangement of corner-sharing alternating BO_6 and $B'O_6$ units are functional materials that have been extensively studied and are suitable for many applications, especially new magnets. For instance, Sr_2FeMoO_6 is a half-metallic ferromagnet (T_C = 415 K) showing colossal magnetoresistance, and Sr_2CrOsO_6 exhibit ferrimagnetic ordering up to very high temperatures (T_C = 725 K).

There are several representatives of double perovskites of the type A_2BIrO_6 (B = trivalent metal) containing Iridium in the formal oxidation state +5. The combination $SrLaBB'O_6$ gives the possibility to combine divalent transition metal ions with Ir^{5+}. By this approach, we were able to synthesize the new compounds $SrLaNiIrO_6$ and $SrLaCuIrO_6$. The first compound crystallizes monoclinically, whereas the second material presents higher tetragonal symmetry with significant Jahn-Teller distortion in the coordination sphere of the $3d^9$ ion Cu^{2+}. Both compounds show isolating behavior. Electronic transport and magnetic data of the powder samples will be presented.

TT 19.29 Mon 15:00 P2-EG

The α-$RuCl_3$ honeycomb system: magnetic anisotropy, high field torque magnetometry and Li- intercalation — •Michael Baenitz[1], Christof Haas[2], Kimberly Modic[1], Mayukh Majumder[1], Hiroshi Yasuoka[1], Helge Rosner[1], Alexander Tsirlin[2], Ernst Wilhelm Scheidt[2], Wolfgang Scherer[2], and Markus Schmidt[1] — [1]MPI for the Chemical Physics of Solids, 01187 Dresden, Germany — [2]Institut fuer Physik, Universitaet Augsburg, 86135 Augsburg, Germany

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 (HKM) was successfully applied for the competing bond-dependent exchange interactions in the 5*d*-honeycomb iridates. 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 ($5d^5$). α-Ru trichloride exhibit a strong magnetic anisotropy evidenced from specific heat and magnetization measurements on single crystals [1]. Here we present torque magnetometry in fields up to 65 T combined with angular dependent magnetization measurements in fields up to 7 T on highly pure single crystals. Furthermore we succeeded in the intercalation of Li into the α-$RuCl_3$ lattice which leads to a suppression of the 8K magnetic order and a reduction of the Curie Weiss moment. Reducing the valency of Ru 3+ towards the 2+ state is rather interesting and opens up a new route to tune this qunatum magnet towards the spin liquid state.

[1] M. Majumder et al. PRB 91 (2015)

TT 19.30 Mon 15:00 P2-EG

Crystal growth and magnetic characterization of kagome-type materials — •Christian Klein[1], Ranjith Kumar[2], Mahmoud Abdel-Hafiez[1], Michael Baenitz[2], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-University, D- 60438 Frankfurt am Main, Germany — [2]Max-Planck-Institute for Chemical Physics of Solids, D-01187 Dresden, 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 spin-1/2 antiferromagnet material Barlowite ($Cu_4(OH)_6BrF$), which represents a model system 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].

Crystals were grown under hydrothermal conditions. Characterization of the samples was done by magnetic measurements to determine the susceptibility and magnetic ordering. Furthermore heat capacity measurements were performed to investigate phase transitions and ordering effects at low temperature.

[1] P. A. Lee, Science 321, 1306 (2008).
[2] T.-H. Han et al., Phys. Rev. Lett. 113, 227203 (2014).
[3] S. Chu et al., Appl. Phys. Lett. 98, 092508 (2011).

TT 19.31 Mon 15:00 P2-EG

Optical conductivity of Na_2IrO_3 supporting the j=1/2 scenario — •Philipp Warzanowski[1], Nick Borgwardt[1], Maria Hermanns[2], Petra Becker[3], Paul van Loosdrecht[1], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für theoretische Physik, Universität zu Köln — [3]Abteilung Kristallographie, Institut für Geologie und Mineralogie, Universität zu Köln

Na_2IrO_3 is widely discussed as a realization of the Heisenberg-Kitaev model with local j=1/2 moments. Challenging the j=1/2 scenario, a description in terms of quasimolecular orbitals (QMOs) with electrons delocalized over individual Ir_6 rings has been suggested [1]. Our infrared transmittance data in the vicinity of the gap for electron-hole excitations provide a litmus test for the underlying microscopic physics, since theoretical predictions based on either QMOs [2] or local j=1/2 moments [3] disagree strongly on the spectral weight of the lowest optical excitation band. We find that the spectral weight below about 0.7 eV is much smaller than reported previously, supporting the j=1/2 scenario. Moreover, we reveal a series of small absorption features around the onset of electron-hole excitations, pointing towards a mixing of electron-hole excitations with local spin-orbital excitations.

[1] I.I. Mazin *et al.*, Phys. Rev. Lett. 109, 197201 (2012)
[2] Y. Li *et al.*, Phys. Rev. B 91, 161101(R) (2015)
[3] B.H. Kim, G. Khaliullin, and B.I. Min, Phys. Rev. B 89, 081109(R) (2014)

TT 19.32 Mon 15:00 P2-EG

Pressure control of quantum magnets with heavy transition-metals — •Marian Blankenhorn[1], Tomohiro Takayama[2], Kentaro Kitagawa[3], Carl Förderer[1], and Hidenori Takagi[1,2,3] — [1]University of Stuttgart, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]University of Tokyo, Tokyo, Japan

Recently, exotic quantum magnetism has been reported in $4d$ and $5d$ transition-metal oxides such as iridates, where the interplay of electron correlation and strong spin-orbit coupling leads to unconventional magnetic coupling. Such $4d$ and $5d$ oxides are regarded as weak Mott insulators produced by modest Coulomb interaction. We expect a pressure induced metal-insulator transition in a moderate pressure range, which may give rise to exotic metallic states and possible superconductivity at the critical point. One of the target materials is the 3-dimensional quantum spin liquid $Na_4Ir_3O_8$, which comprises a hyper-kagome lattice of Ir^{4+}-ions. $Na_4Ir_3O_8$ is known to be tuned into a metal by carrier doping and thus we expect that $Na_4Ir_3O_8$ can be driven into a metallic state by applying pressure. We also study honeycomb-based oxides, which are candidates for quantum spin liquids.

In order to apply high pressure up to 10 GPa, we use an opposed-anvil high pressure cell developed by Kitagawa et al. allowing electric transport measurements. We report preliminary pressure-studies on these heavy transition-metal quantum magnets and discuss the nature of exotic metallic states expected under high pressure.

TT 19.33 Mon 15:00 P2-EG

ESR study of the triangular-lattice antiferromagnet Cs_2CuBr_4 — •E. Schulze[1,2], A. N. Ponomaryov[1], J. Wosnitza[1,2], H. Tanaka[3], and S. A. Zvyagin[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Department of Physics, Tokyo Institute of Technology, Japan

We present high-field electron spin resonance (ESR) studies of the spin-1/2 triangular-lattice antiferromagnet Cs_2CuBr_4. The temperature dependences of ESR parameters (the effective g factor and ESR linewidth) were measured for magnetic fields applied along the three principal directions. From the angular dependence of the ESR linewidth the Dzyaloshinskii-Moriya interaction was estimated. The results are compared with the data obtained on the isostructural compound Cs_2CuCl_4.

TT 19.34 Mon 15:00 P2-EG

Density matrix embedding theory for multi-band Hubbard models — •Michael Schmid and Maria Daghofer — Universität Stuttgart

Density matrix embedding theory (DMET) [1], a recently proposed numerical method when working on many-particle systems, and its cluster formulation (CDMET) [2] are used to investigate strongly correlated electron systems such as multi-band Hubbard models. Firtst the method is tested for the single-band Hubbard model in one and two dimensions. Then we extend the method, which so far was just used to study single-band systems, to multi-band systems. We hope to get further insight into the two-band Hubbard model on a cubic lattice by using an exact diagonalization solver.

[1] G. Knizia et. al., Phys. Rev. Lett. 109, 186404 (2012)
[2] B. Zheng et. al., arXiv preprint arXiv:1608.03316 (2016)

TT 19.35 Mon 15:00 P2-EG

X-ray absorption in strong correlated high T_C superconductors — •Tobias Pitters and Maria Daghofer — Institut für Funktionelle Materie und Quantentechnologien

In X-ray absorption spectroscopy, a possible process is to create a core hole an add the electron to the valence states. Theoretically, this can be treated by evaluating the one-particle Green's function in the presence of a strong potential. When modelling the antiferromagnetic parent state of high-T_C cuprate superconductors, the potential can be onsite or situated between two neighboring sites. We analyze this problem for parameter regimes relevant to cuprates and iridates using the self-consistent Born approximation.

TT 19.36 Mon 15:00 P2-EG

Variational Cluster Approximation for Spin Liquids — •Teresa Schaller and Maria Daghofer — Institut für funktionelle Materie und Quantentechnologien, Universität Stuttgart, Deutschland

We use the variational cluster approximation to investigate the phase diagram and one-particle spectral density of multi-band Hubbard models. The approach includes quantum fluctuations on a small cluster exactly and long-range order on a mean-field level. We will in particular investigate the filling of five electrons in the t_{2g} subshell, as it is realized in some iridium compounds. The interaction of Hund's rule and spin-orbit coupling leads to various magnetic orderings in the ground state. We present the phase diagram resulting from this competition and the impact of crystal-field splitting.

TT 19.37 Mon 15:00 P2-EG

Mean-field extension of the variational cluster approach — •Jan Lotze and Maria Daghofer — Universität Stuttgart, Institut für Funktionelle Materie und Quantentechnologien, Pfaffenwaldring 57, 70550 Stuttgart

The variational cluster approximation (VCA) based on self-energy functional theory (SFT) can be used to study correlated-electron Hamiltonians: Instead of the original systems self-energy, that of a 'reference system' is considered. Both systems must share the same two-body interactions, but may differ in one-body terms such as the kinetic hopping. Within VCA, the reference system is formed by isolated clusters. From the SFT perspective, inter-site interactions cannot be included. We propose to incorporate interactions along bonds inside the clusters exactly, while those between clusters are mean-field decoupled. Although this is an approximation, it should be controlled by the cluster-size as for pure VCA.

Results obtained for the extended Hubbard model in one and two dimensions on a square [1] and a honeycomb lattice [2] are shown.

[1] M. Aichhorn, H. G. Evertz, W. von der Linden and M. Potthoff, Phys. Rev. B **70**, 235107 (2004)
[2] M. Daghofer and M. Hohenadler, Phys. Rev. B **89**, 035103 (2014)

TT 19.38 Mon 15:00 P2-EG

Disordered Weyl spin liquids — •Kevin O'Brien, Maria Hermanns, and Simon Trebst — Universität zu Köln

Electronic Weyl semimetals have garnered considerable attention since their recent observation in TaAs and photonic materials. Here we investigate the spin analogue of the electronic Weyl semimetal – the *Weyl spin liquid*.

Such a state can be readily found in generalizations of the Kitaev honeycomb model on certain three-dimensional tricoorinated lattices. In these Weyl spin liquids, the original spin-1/2 moments form a quantum spin liquid wherein they fractionalize into gapped flux excitations of a Z2 gauge field as well as into Majorana fermions which form the gapless Weyl dispersion. One unusual aspect of the Weyl spin liquid is that it may appear under symmetry conditions which would forbid the formation of its conventional electronic counterpart, namely, with both time-reversal and inversion symmetry intact.

In this work we discuss some general properties of Weyl spin liquids as well as the impact of disorder. In particular, we investigate the effects of short- and long-range correlated disorder on the low-energy physics of these systems, and to what extent disorder is sensitive to the underlying symmetry class.

TT 19.39 Mon 15:00 P2-EG

Thermodynamics of spin fractionalization in Kitaev matter — •Tim Eschmann and Simon Trebst — Institute for Theoretical Physics, University of Cologne

The fractionalization of quantum numbers is one of the most intriguing phenomena in quantum many-body systems. Here we study the thermodynamic signatures of spin fractionalization in Kitaev models in two and three spatial dimensions by means of numerically exact quantum Monte Carlo techniques. Analytically, the fractionalization of the original spin degrees of freedom into itinerant Majorana fermions and a static $\mathbb{Z}_2$ gauge field is well understood at zero temperature and has led to a comprehensive classification of the emergent Majorana metals for a variety of two and three-dimensional lattices relevant to a number of spin-orbit dominated materials. Here, we put our focus on the physics of the $\mathbb{Z}_2$ gauge field and discuss the finite-temperature phase transitions associated with the ordering of the gauge field in three spatial dimensions.

TT 19.40 Mon 15:00 P2-EG

Spin liquids and competing magnetic orders in three-dimensional kagome magnets — •Finn Lasse Buessen and Simon Trebst — University of Cologne, Germany

One of the best experimentally established spin liquids is found in the

hyperkagome compound Na4Ir3O8 where geometric frustration is an inherent feature of its three-dimensional lattice structure of corner-sharing triangles. Here we present a detailed numerical analysis of these systems in the presence of competing nearest and next-nearest neighbor interactions using a recently developed pseudo-fermion functional renormalization group (pf-FRG) approach. We discuss why this approach allows to access the strong-coupling regime of quantum spin systems, highlight technical aspects of a state-of-the-art numerical implementation, and demonstrate its applicability for the hyperkagome systems and other three-dimensional frustrated quantum magnets.

TT 19.41 Mon 15:00 P2-EG

Spectral function of a quantum dimer model for the pseudogap metal — •Sebastian Huber and Matthias Punk — Arnold Sommerfeld Center, Ludwig-Maximilians University, 80333 Munich, Germany

We study a quantum dimer model [1,2], which describes several key properties of the pseudogap phase of hole-doped cuprates at low hole density p. The configurations of the system are built from two species of dimers: Fermionic dimers that carry spin S = 1/2 and charge +e embedded in a neutral background of bosonic spin singlet dimers.
We compute electron spectral functions using exact diagonalization on lattices of size 6x6 and find clear signature of the so-called pseudogap at the antinode in momentum space.
In a second part we show how to implement a cluster dynamical mean-field approach in order to calculate spectral properties of the quantum dimer model with higher resolution. The cluster impurity problem is solved using the numerical renormalization group technique.

[1] D. S. Rokhsar and S. A. Kivelson, PRL 61, 20 (1988)
[2] M. Punk, A. Allais and S. Sachdev, PNAS 112, 31 (2015)

TT 19.42 Mon 15:00 P2-EG

Dynamics of a triangular spin-ladder with ring exchange — •Jonas Richter and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

Ring exchange processes which become non-negligible in weak Mott insulators, typically enhance magnetic frustration and may lead to novel physics. Using linear response theory, we study the finite temperature spin and current dynamics of a triangular two-leg spin ladder with additional four-spin ring exchange which can potentially be viewed as a one-dimensional descendent of the organic Mott insulator κ-$(ET)_2Cu_2(CN)_3$. Employing complementary numerical methods, namely exact diagonalization, the Lanczos algorithm and dynamical quantum typicality, we present results for the static and dynamic structure factor, spin and energy conductivities and their corresponding Drude weights. We explore the relevant parameter space, both into the spin-Peierls as well as into the putative spin-Bose metal phase and uncover unique features in the spin dynamics which are not present for nearest-neighbor Heisenberg exchange only.

TT 19.43 Mon 15:00 P2-EG

Thermal transport in the Kitaev spin model — •Angelo Pidatella[1], Alexandros Metavitsiadis[2], and Wolfram Brenig[2] — [1]Institute for Theoretical Physics, Technical University of Dresden — [2]Institute for Theoretical Physics, Technical University of Braunschweig

We analyze the dynamical thermal conductivity of the Kitaev spin model on the honeycomb lattice, which constitutes an exactly solvable example for a Z_2 spin liquid. Using a mapping to Majorana particles, the thermal transport is described in terms of matter fermions interacting with a Z_2 gauge field. Findings for the transport coefficient within linear response theory will be discussed in the long wave length limit, at finite frequency, and arbitrary temperature. For the zero flux sector, analytic results will be presented, while finite flux densities will be treated numerically within a real space approach, invoking either a summation over all gauge sectors, or using an average gauge field configuration approach. Comparison with findings for the thermal transport in Kitaev spin ladders will also be provided.

TT 19.44 Mon 15:00 P2-EG

The spin-1/2 Kagome XXZ model in a field: competition between lattice nematic and solid orders — •Augustine Kshetrimayum[1], Thibaut Picot[2], Román Orús[1], and Didier Poilblanc[2] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Laboratoire de Physique Théorique, IRSAMC, CNRS and Université de Toulouse, UPS, F-31062 Toulouse, France

We study numerically the spin-1/2 XXZ model in a field on an infinite Kagome lattice. We use different algorithms based on infinite Projected Entangled Pair States (iPEPS) for this, namely: (i)an approach with simplex tensors and 9-site unit cell, and (ii) an approach based on coarse-graining three spins in the Kagome lattice and mapping it to a square-lattice model with local and nearest-neighbor interactions, with usual PEPS tensors, 6- and 12-site unit cells. We observe the emergence of several magnetization plateaus as a function of the field for different values of the anisotropy. We focus on the 1/3 plateaus using both the techniques and study the nature of its ground state as we tune the anisotropy from the Ising regime to the XY regime through the Heisenberg point and find a strong competition between lattice nematic and solid orders.

TT 19.45 Mon 15:00 P2-EG

Topological domain walls in helimagnets — •Laura Köhler[1], Jan Müller[2], Achim Rosch[2], Peggy Schönherr[3], Dennis Meier[3,4], and Markus Garst[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, 50937 Cologne, Germany — [3]Department of Materials, ETH Zürich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland — [4]Department of Materials Science and Engineering, Norwegian University of Science and Technology, 7491 Trondheim, Norway

A magnetic helix arises in chiral magnetic materials with a wavelength set by the spin-orbit coupling. Using micromagnetic simulations and comparing to experimental studies on surfaces of FeGe, we show that domain walls of such helimagnetic order are distinctly different from ferromagnets and rather similar to grain boundaries of liquid crystals. Three types of domain walls are realized depending on the relative domain orientation: a curvature wall, a zig-zag disclination wall and a dislocation wall. Disclinations are vortex defects in the helix axis orientation, and they can be combined to form dislocations. We discuss the topological skyrmion charge associated with these defects, and we demonstrate that domain walls of helimagnetic order can carry a finite topological charge on average. As a consequence, they can be manipulated by spin currents and contribute to a topological Hall effect.

TT 19.46 Mon 15:00 P2-EG

Fermi surfaces of B20 compounds from Density Functional Theory and de Haas-van Alphen effect — Schorsch Michael Sauther[2], •Arthur Niedermayr[1], Matthias Dodenhöft[4], Andreas Bauer[1], Frank Freimuth[3], Bernd Zimmermann[3], Yuriy Mokrousov[3], Dirk Grundler[5], Christian Pfleiderer[1], and Marc Andreas Wilde[1] — [1]Phys.-Dep. E51, TU München — [2]Phys.-Dep. E10, TU München — [3]Peter Grünberg Institute, Jülich — [4]Phys.-Dep. E21, TU München — [5]LMGN, Lausanne

The class of chiral intermetallic compounds with cubic B20 crystal structure have attracted a lot of interest. Manganese silicide (MnSi) is a metal known for its unusual magnetic properties including a skyrmion lattice phase as well as for its strong electronic correlations and non-Fermi liquid behavior under pressure. The isostructural iron silicide (FeSi), on the other hand is commonly assumed to be a strongly correlated small-gap semiconductor at low temperature. However, the nature of the insulating state and the role of the crystal surface are not yet fully settled. We combine density functional theory (DFT) calculations and the de Haas-van Alphen (dHvA) effect in order to investigate the electronic properties of B20 compounds. First results indicate a substantial role of spin-orbit coupling for the Fermi surface properties of MnSi.

TT 19.47 Mon 15:00 P2-EG

Optical conductivity of layered ruthenates: spin-orbit and anistropic Coulomb interaction effects — •Esmaeel Sarvestani, Guoren Zhang, Evgeny Gorelov, and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich,D-52425 Jülich, Germany

Using the LDA+DMFT approach, we calculate the in-plane and out-of-plane optical conductivity of the single-layered (Sr_2RuO_4) and double-layered ($Sr_3Ru_2O_7$) ruthenates. The calculations are performed via linear response theory and Kubo's formalism. We investigate the effects of the electron-electron interaction, the spin-orbit coupling and the low-symmetry Coulomb interaction in the optical spectra. We show that including the spin-orbit coupling improves the agreement with experimental data while the anisotropic Coulomb interaction does not change the in-plane optical spectrum. We find that, contrary to the out-of-plane conductivity, the in-plane conductivity changes con-

siderably by changing temperature and Coulomb interaction and by including the spin-orbit coupling. We explain the difference in behaviour of the in-plane and out-of-plane conductivities in terms of the corresponding non-interacting transport functions. Furthermore, we discuss the effective mass-enhancement and quasi-particle scattering rate.

TT 19.48 Mon 15:00 P2-EG

Crystal structure determination of Ti-doped Ca_2RuO_4 — •Sebastian Hoffmann, Stefan Kunkemöller, Kevin Jenni, and Markus Braden — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln, Germany

The crystal structure of 0, 1 and 10% Ti-doped Ca_2RuO_4 was determined by single crystal X-ray diffraction at 100K and 300K. To clarify the mechanism of superconductivity in Sr_2RuO_4, the phase diagram of $Ca_{2-x}Sr_xRuO_4$ was analysed, which possesses ferromagnetism, anitferromagnetism, superconductivity, orbital ordering and metal-insulator transitions. Sr_2RuO_4 is isostructural to the ideal tetragonal K_2NiF_4 structure with spacegroup $I4/mmm$ and non-distorted NiF_6-octahedra. The Mott insulator Ca_2RuO_4 crystallizes in the orthorhombic spacegroup $Pbca$, in which the RuO_6-octahedra are highly distorted. Upon cooling, structural changes lead to effects like the anomalous elongation of the b-lattice constant and to a shortening of the a- and c-lattice constant. These changes are accompanied by a flattening, rotation and tilting of the RuO_6-octahedra, with the tilt occuring around the b-lattice constant. In Ca_2RuO_4 there seems to be a connection of the magnetic ordering at low temperatures and the structural behaviour. Upon cooling below 110K, where antiferromagnetic order sets in, the elongation of the b-lattice constant saturates. Ti doping up to 10% seems to change the elongation from $b(300K) - b(T_N) = 0.1643$Å down to 0.0898Å. For the Ti-doped samples, the anomalous properties of Ca_2RuO_4 (relative to Sr_2RuO_4) are thus attenuated.

TT 19.49 Mon 15:00 P2-EG

Crystal growth of Ti-doped perovskite ruthenates — •Kevin Jenni, Sebastian Hoffmann, Stefan Kunkemöller, and Markus Braden — II. Physikalisches Institut, Universität zu Köln

Ruthenates of the Ruddlesden-Popper series exhibit a variety of interesting phenomena ranging from unconventional superconductivity in Sr_2RuO_4 to the Mott-insulating state in Ca_2RuO_4. Titanium doping has been found to alter dramatically the physical properties of these materials. By partially replacing the Ruthenium in the Oxygen octahedra by nonmagnetic four-valent Titanium magnetic fluctuations can be stabilized which leads to a SDW ordering in $Sr_2Ru_{0.91}Ti_{0.09}O_4$ or $Sr_3(Ru_{0.91}Ti_{0.09})_2O_7$. In $Ca_{1.78}Sr_{0.22}Ru_{0.9}Ti_{0.1}O_4$ a metal-insulator phase transition can be observed around 80 K in contrast to the undoped sample which is metamagnetic. However the availability of ruthenate crystals is limited because the growth is challenging due to the high evaporation of ruthenium up to 90% and the intergrowth of different layered ruthenates. Therefore the determination of exact growth parameters is crucial. We present the growth of single crystals of $Ca_{1.78}Sr_{0.22}Ru_{1-x}Ti_xO_4$ and $Ca_{2-x}Sr_xRuO_4$. The crystal growth was conducted by travelling floating-zone method using a Canon SC1-MDH mirror furnace yielding large crystals.

TT 19.50 Mon 15:00 P2-EG

Giant Magnetostriction, structural domain switching, and anomalous Hall effect on untwinned $SrRuO_3$ single crystals — •Danie Brüning, Stefan Kunkemöller, Markus Braden, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Deutschland

$SrRuO_3$ is the infinite-layer material of the well-known Ruddlesden-Popper series of ruthenates $Sr_{n+1}Ru_nO_{3n+1}$, which have attracted enormous interest not only due to the unconventional superconductivity in Sr_2RuO_4. Ruthenates show a large variety of physical phenomena due to electronic correlations and spin-orbit coupling. $SrRuO_3$ is the only ferromagnetic metal in this series. It is heavily studied as a conducting perovskite layer in thin films. Despite the big interest in the research of $SrRuO_3$ large and high quality single crystals became available only very recently. Our high quality cm^3 size single crystals are grown with the optical floating zone technique. From the high temperature cubic phase $SrRuO_3$ becomes tetragonal and orthorhombic via two transitions which allows for 6 twins. With uniaxial pressure applied upon cooling it is possible to untwin these crystals. We present investigations on the switching of the different structural domain states linked to a giant magnetostriction. Additionally, we analyze the anomalous Hall effect of $SrRuO_3$ and the anisotropy gap in the magnon dispersion.

Supported by the DFG via CRC 1238.

[1] S. Kunkemöller et al., Crys. Res. and Technol., 51: 299 (2016)

TT 19.51 Mon 15:00 P2-EG

"Ferroelectric" phase transition in conducting $Sr_{1-x}Ca_xTiO_{3-\delta}$ — •Dennis Finck, Steffen Harms, Xiao Lin, Christoph P. Grams, Johannes Engelmayer, Thomas Lorenz, and Joachim Hemberger — II. Physikalisches Institut, Universität zu Köln, Germany

Insulating $SrTiO_3$ is a so-called quantum paraelectric close to an ferroelectric instability. On the one hand, the substitution of strontium ions by smaller and isovalent calcium ions induces a ferroelectric phase at finite temperatures. On the other hand, $SrTiO_3$ becomes metallic and even superconducting at temperatures below 1K after charge carrier doping [1].

Therefore the question arises what happens when both effects are combined. Here, we provide experimental evidence for a polar ground state also in the metallic compound. As mobile charge carriers screen the electric polarization, it is technically not possible to directly measure ferroelectricity. Thus, our conclusion ist based on measurements of sound velocities and thermal expansions.

Funded through the Institutional Strategy of the University of Cologne within the German Excellence Initiative.

[1] B. S. de Lima, M. S. da Luz, F. S. Oliveira, L. M. S. Alves, C. A. M. dos Santos, F. Jomard, Y. Sidis, P. Bourges, S. Harms, C. P. Grams, J. Hemberger, X. Lin, B. Fauqué, and K. Behnia,
Phys. Rev. B **91**, 045108 (2015)

TT 19.52 Mon 15:00 P2-EG

Impact of electron doping on thermodynamic and transport properties of the magnetoelectric antiferromagnet $EuTiO_{3-\delta}$ — •Johannes Engelmayer, Christoph Grams, Xiao Lin, Joachim Hemberger, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Germany

Various perovskite titanates $ATiO_3$ are known to undergo ferroelectric phase transitions, e.g., for $A = \mathrm{Ba, Pb, Cd}$. In contrast, $CaTiO_3$ and $SrTiO_3$ show quantum paraelectric behavior, that is, ferroelectric long-range order is suppressed by quantum fluctuations. In addition, the insulating $SrTiO_3$ becomes metallic upon electron doping via oxygen deficiencies ($SrTiO_{3-\delta}$ with $\delta > 0$) and even shows superconductivity for certain carrier concentrations. The rare-earth titanate $EuTiO_3$ is similar to $SrTiO_3$. Both, Eu^{2+} and Sr^{2+} have the same ionic radii, but Sr^{2+} is nonmagnetic while Eu^{2+} has a large magnetic moment of $7\mu_B$. Below $T_N = 5.5$ K the localized 4f moments order antiferromagnetically in a G-type configuration. While stoichiometric $EuTiO_3$ is semiconducting, metallic behavior can be induced by oxygen deficiencies, similar to $SrTiO_{3-\delta}$. Here, we present a detailed characterization of $EuTiO_{3-\delta}$ with $-10^{-2} \leq \delta \leq 10^{-2}$ based on field- and temperature-dependent measurements of magnetization, specific heat, and thermal expansion. Moreover we use resistivity and permittivity measurements as complementary methods to investigate the magnetoelectric properties, since the conductivity of the samples covers 17 orders of magnitude.

TT 19.53 Mon 15:00 P2-EG

Correlating paramagnetic spin centers in the 'nonmagnetic' $5d^4$ compound Ba_2YIrO_6 — •Stephan Fuchs[1], Vladislav Kataev[1], Franziska Hammerath[1], Gizem Aslan Cansever[1], Tushar Dey[1], and Bernd Büchner[1,2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden,D-01171 — [2]Institut für Festkörperphysik, Technische Universität Dresden,D-01062

We will present the electron spin resonance results of the double perovskite Ba_2YIrO_6. This material provides a playground to examine the magnetic interactions in a 5d transition metal oxide with strong spin-orbit coupling. Theory predicts that due to the strong spin-orbit coupling this $5d^4$ iridate should be in a nonmagnetic state. However, static magnetic and NMR measurements evidence the occurrence of paramagnetic spin centers that are correlated at low temperatures. To obtain deeper insight into the magnetic properties of Ba_2YIrO_6 ESR measurements of a polycrystalline sample were carried out for several temperatures and frequencies. This enables to quantify several different paramagnetic spin centers. Two of them correspond to S=1/2 with the g-factor g=1.99 and g=1.90, and the third one to S=3/2 with g=1.49. An overview of the possible origins for the different spin cen-

ters and their relevance to the unexpected magnetism of this compound will be shown on this poster.

TT 19.54 Mon 15:00 P2-EG

NMR Investigation of Ir-based Double Perovskites — •Margarita Iakovleva[1,2,3], Evgeniia Vavilova[3], Hans-Joachim Grafe[1], Manna Kaustuv[4], Michael Vogl[1,2], Tusharkanti Dey[5], Sabine Wurmehl[1], Bernd Büchner[1,2], and Vladislav Kataev[1] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Zavoisky Physical-Technical Institute, Kazan, Russia — [4]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [5]Universität Augsburg, Augsburg, Germany

Iridium based double perovskites are unique materials where Coulomb repulsion, strong spin-orbit coupling, exchange interaction and crystal field have comparable energy scales. The interplay between all of these interactions and correlations may lead to the emergence of novel electronic and magnetic states. In this work we report the ^{139}La nuclear magnetic resonance (NMR) results on the double perovskite compounds La_2MIrO_6 with magnetic and nonmagnetic ions at the M position (M = Co, Cu, Zn). Nuclear relaxation rate ${T_1}^{-1}$ measurements in La_2CuIrO_6 show the peak at $T \approx 74$ K that is the signature of a magnetic transition. Moreover with further decreasing the temperature the T-dependence of ${T_1}^{-1}$ shows the shoulder at $T \approx 60$ K that can be associated with a cooperative ordering of the transverse moments. In case of La_2CoIrO_6 the ${T_1}^{-1}$ measurements do not show any anomalies at T below the ordering temperature. Our investigation has revealed complex magnetic interactions in the compound where strongly spin-orbit coupled 5d transition metal ions coexist with strongly correlated spin-only 3d (Co, Cu) and non-magnetic Zn ions.

TT 19.55 Mon 15:00 P2-EG

Microstructuring Quantum Materials — •Toni Helm, Maja Bachmann, Kimberly Modic, Kent Shirer, Markus König, Sebastian Seifert, Nabhanila Nandi, Andrew Mackenzie, and Philip Moll — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

In 'Quantum materials', non-trivial quantum mechanics leads to unusual physical properties that promise the potential to improve our understanding of many body quantum states as well as to spark ideas for novel electronic applications exploiting these unusual properties. Our research focuses on the mesoscale physics of quantum matter, in particular topological matter, unconventional superconductors and magnetic metals when their dimensions become comparable to their relevant length scales on the micron and sub-micron level. We develop techniques based on focused ion beam (FIB) micromachining to fabricate mesoscopic devices from single crystals. We showcase three examples of the wide range of materials and applications approachable by microstructuring: We show (1) how Fermi arc surface states contribute to the charge transport in microstructures of the Dirac semimetal Cd_3As_2 on length scales smaller than the mean-free-path; (2) how a subtle phase transition just above the superconducting transition changes the electronic structure in the quasi-1D metal $Ta_4Pd_3Te_{16}$, revealed by resistivity anisotropy measurements on the micron-scale and (3) how micro-channels of ultra-pure metals with electron-electron scattering such as $PdCoO_2$ can lead to hydrodynamic corrections to the standard ballistic transport.

TT 19.56 Mon 15:00 P2-EG

Cantilever-based torque magnetometry for de Haas-van Alphen experiments on correlated metals — •Marc Andreas Wilde, Schorsch Michael Sauther, Arthur Niedermayr, Andreas Bauer, and Christian Pfleiderer — Physik Department, Technische Universität München, James-Franck-Strasse 1, 85748 Garching, Germany

Cantilever-based torque magnetometers have been optimized to measure the quantum oscillations of the magnetization, i.e., the de Haas-van Alphen (dHvA) effect in both correlated bulk metals and low-dimensional electron systems. For strongly correlated bulk metals the focus of the sensor and readout design is on a compact, rotatable and Millikelvin-compatible setup that fits into the bore of standard high-field superconducting solenoids. For low-dimensional systems highest sensitivity due to the inherently small signal strength is a prerequisite. We present specific implementations based on capacitive readout and fiber-optical interferometry and discuss their advantages and limitations in the context of dHvA experiments on correlated metals. In particular when large bulk crystals are not available, position readout techniques that do not scale with the sensor size are shown to be advantageous.

TT 19.57 Mon 15:00 P2-EG

Experimental determination of the Fermi surface in transition metal diborides — •Schorsch Michael Sauther[1], Matthias Dodenhöft[1], Matthias Brasse[1], Stephan Gerhard Albert[1], Jan Kuneš[2], Andreas Bauer[1], Alexander Regnat[1], Olga Young[3], Uli Zeitler[3], Christian Blum[4], Sabine Wurmehl[4,5], Dirk Grundler[6], Christian Pfleiderer[1], and Marc Andreas Wilde[1] — [1]Physik-Department, TU München — [2]Institute of Physics, Academy of Sciences, Prag — [3]HFML-EMFL, Radboud University, Nijmegen — [4]IFW, Dresden — [5]Institut für Festkörperphysik, TU Dresden — [6]LMGN, IMX, STI, EPF Lausanne

Transition metal diborides exhibit a variety of ground states including BCS superconductivity and complex forms of magnetic order. For a detailed understanding of the magnetic and electronic properties a comprehensive picture of the Fermi surface (FS) is a prerequsite. For the itinerant antiferromagnet chromium diboride (CrB_2), e.g., the intricate interplay between FS properties and the complicated magnetic order is not yet fully understood [1]. We employ torque magnetometry at low temperatures down to 0.3 K and in high magnetic fields up to 35 T to measure the quantum oscillations of the magnetization, i.e., the de Haas-van Alphen (dHvA) effect. Combined with density functional theory (DFT) calculations, the dHvA effect is a powerful tool that allows determination of the FS properties. We present recent results on CrB_2 and further isostructural diborides.
[1] M. Brasse *et al.*, Phys. Rev. B **88**, 155138 (2013)

TT 19.58 Mon 15:00 P2-EG

Electrochemical Characterization and Valence Tuning of Lithium Nitridometallates — •Elisa Thauer[1], Alex Ottmann[1], Christoph Neef[1], Manuel Fix[2], Anton Jesche[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institut für Physik, Universität Heidelberg, D-69120 Heidelberg, Germany — [2]Experimentalphysik VI, Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

The electrochemical properties of lithium metal nitrides $Li_2Li_{1-x}M_xN$ with M = Fe or Ni and of Li_3N are investigated by cyclic voltammetry and galvanostatic cycling. Based on these results, the lithium content and thus the valence of the transition metal ions is altered electrochemically. In addition to XRD studies on the electrochemically treated materials, the effect of delithiation on the magnetic properties is studied by means of SQUID magnetometry. For $Li_{2.7}Fe_{0.3}N$, electrochemical tuning yields suppression of the initial hard magnetic ground state. In the case of $Li_{2.6}Ni_{0.4}N$, the paramagnetic response diminishes upon delithiation. Finally, we show perspectives for delithiation procedures in Li_3N.

TT 19.59 Mon 15:00 P2-EG

Growth of stoichiometric $LaTiO_3$ thin films by pulsed laser deposition — •Philipp Scheiderer, Matthias Schmitt, Alex Gössmann, Michael Sing, and Ralph Claessen — Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), 97074 Würzburg, Germany

Oxide heterostructures exhibit fascinating properties, e.g., the coexistence of superconductivity and ferromagnetism at the interface of $LaAlO_3/SrTiO_3$, but the extraordinary electronic properties of transition metal oxides (TMOs) caused by electron correlation yet wait to be fully harnessed. The Mott insulator $LaTi^{3+}O_3$ (LTO) is a prototypical material for such strongly correlated TMOs, which can be prepared by pulsed laser deposition. However, in order to obtain stoichiometric LTO strongly reducing growth conditions are required since the thermodynamically stable bulk phase is the oxygen-rich band insulator $La_2Ti_2^{4+}O_7$.
We therefore systematically study the impact of oxidizing and reducing background atmospheres and the oxygen out diffusion from the substrate into thin LTO films. *In situ* x-ray photoelectron spectroscopy of films prepared on STO reveals overoxidation due to oxygen outdiffusion from the STO substrate, which can be partially suppressed by introducing a $LaAlO_{3-x}$ (LAO) buffer layer. Further control over the oxygen stoichiometry is gained by the use of $DyScO_3$ substrates, presumably due to the lower mobility of oxygen. Overoxidation during storage in air can be prevented by introducing a LAO capping layer of a few unit cells thickness, acting again as a diffusion barrier for oxygen.

TT 19.60 Mon 15:00 P2-EG

Synthesis and Characterization of $La_{2-2x}Sr_{1+2x}Mn_2O_7$ thin

films — •Florian Hollemann, Marius Keunecke, Vladimir Roddatis, Daniel Steil, Stefan Mathias, and Vasily Moshnyaga — Georg-August-Universität Göttingen

Perovskite oxides are an intriguing material system showing effects like superconductivity, CMR, metal-insulator transitions. These effects are related to the strong interaction between charge, spin, orbit and lattice degrees of freedom. Because of the inherent 2D structure the layered manganite $La_{2-2x}Sr_{1+2x}Mn_2O_7$ is attractive as a model system for low-dimensional physics and can serve as a playground to study these interactions. We fabricated Ruddlesden-Popper phase (n=2) $La_{2-2x}Sr_{1+2x}Mn_2O_7$ thin films on LSAT(001) substrates using metalorganic aerosol deposition (MAD), with and without atomic layer epitaxy (ALE). For bulk systems the phase diagram is well known, but for thin films it is not yet completely reported. Our aim is to develop a thin film phase diagram by varying the doping x and characterising the electrical and magnetic behavior by using SQUID and PPMS. The structural quality and phase purity was checked using the in-situ-ellipsometry, XRR, XRD, AFM and TEM.

TT 19.61 Mon 15:00 P2-EG

Emergence of hydrodynamic long-time tails from noisy Boltzmann equations — •Philipp Weiss, Jonathan Lux, and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

When an interacting quantum system undergoes a quantum quench, we expect that the system will ultimately reach thermal equilibrium. Local equilibrium is established by scattering of quasiparticles on intermediate time scales. However, global equilibration requires diffusive transport of conserved quantities resulting in a slow algebraic relaxation towards thermal equilibrium. Phenomenologically, the final state of the relaxation can be described by fluctuating hydrodynamics. But, how does this irreversible dynamics emerge from the unitary time-evolution of a closed quantum system?

Here, we address this question within a quantum-kinetic approach. Even on the level of the Boltzmann equation an additional noise term is required to reproduce the algebraic long-time behavior. In a first step, we show that fluctuating hydrodynamics can be derived from the fluctuating Boltzmann equation. Similarly, we aim to derive a "noisy quantum-Boltzmann equation" which mimics the hydrodynamic fluctuations on the quantum level. A possible derivation starts from a modified Keldysh-Dyson equation, supplemented by a noise term. Such an equation defines a noise-dependent Green's function. Following this route, we have to ensure that averaging of "noisy Green's functions" reproduces the exact higher-order correlation functions.

TT 19.62 Mon 15:00 P2-EG

Pumping approximately integrable systems — •Florian Lange, Zala Lenarcic, and Achim Rosch — Universität zu Köln

Weak perturbations can drive an interacting many-particle system far from its initial equilibrium state if one is able to pump into degrees of freedom approximately protected by conservation laws. This concept has for example been used to realize Bose-Einstein condensates of photons, magnons, and excitons. Integrable quantum systems like the one-dimensional Heisenberg model are charac- terized by an infnite set of conservation laws. Here we develop a theory of weakly driven integrable systems and show that pumping can induce huge spin or heat currents even in the presence of integrability breaking perturbations, since it activates local and quasi-local approximate conserved quantities. The resulting steady state is qualitatively captured by a (truncated) generalized Gibbs ensemble with Lagrange parameters that depend on the structure but not on the overall ampli- tude of perturbations or on the initial state. We suggest to realize novel heat or spin pumps using spin-chain materials driven by THz radiation.

TT 19.63 Mon 15:00 P2-EG

A simple tensor network algorithm for 2d steady states — •Augustine Kshetrimayum[1], Hendrik Weimer[2], and Román Orús[1] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Insitut für Theoretische Physik, Leibniz Universität Hannover, AppelStrasse 2, 30167 Hannover, Germany

We present a tensor network algorithm that approximates steady-states of 2d quantum lattice dissipative systems in the thermodynamic limit. The implementation of our method is remarkably simple and efficient. We prove the validity of the approach by computing the steady states of a dissipative quantum Ising model, relevant to address controversies in dissipative systems of interacting Rydberg atoms, and benchmark our simulations with a variational algorithm based on product and correlated states. Our method is the first implementation of the calculation of steady states in 2d for quantum lattice systems with tensor networks.

TT 19.64 Mon 15:00 P2-EG

Real-time dynamics in the two-dimensional Kondo-lattice model with classical spins — •Lena-Marie Gebauer — I. Institut für Theoretische Physik, Universität Hamburg

The two-dimensional ferromagnetic Kondo lattice with localized spins coupled to a system of non-interacting conduction electrons is the prototypical model for layered manganites and can be simulated using ultracold fermions trapped in optical lattices. Here, we present a quantum-classical hybrid theory for the thermodynamics and the real-time dynamics of the model where the spins are treated as classical degrees of freedom.

The equilibrium phase diagram is derived and found to agree well with previous classical Monte-Carlo data [2]. It comprises different phases, an antiferromagnet at half-filling as well as ferromagnetic, incommensurate and phase-separated states. We study the exact real-time dynamics initiated by different parameter quenches.

[1] M. Sayad, M. Potthoff, New J. Phys. 17 (2015) 113058
[2] S. Yunoki et al., Phys. Rev. Lett. 80, 845 (1998)

TT 19.65 Mon 15:00 P2-EG

First-principles molecular transport calculation — •Michael Rumetshofer, Gerhard Dorn, Lilia Boeri, Enrico Arrigoni, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

We have performed a first-principles calculation of the charge transport through a benzene-1,4-dithiol (BDT) molecule contacted by two semi-infinite gold chains. Density Functional Theory, within the plane-wave pseudopotential method, is used to calculate the electronic band structure. Transforming the Kohn-Sham eigenvalues and eigenfunctions to a real-space basis of maximally localized Wannier functions allows extracting a tight-binding Hamiltonian to describe the transport system. Strong electron correlations are included on the BDT molecule using an extended Hubbard model, similar to [1]. Non-equilibrium Green functions are then used to calculate the charge transport through the BDT molecule. It turns out that in the case of single gold chains as leads, the transport properties are determined only by the orbitals coupling to the gold s-orbitals. Therefore transport through the benzene p_z-orbitals is suppressed.

[1] D. A. Ryndyk, A. Donarini, M. Grifoni, K. Richter, Phys. Rev. B 88, 085404 (2012).

TT 19.66 Mon 15:00 P2-EG

Non-equilibrium steady states of the ionic Hubbard model in strong electric fields — •Yusuf Mohammed and Martin Eckstein — Max Planck Research Department for Structural Dynamics, Hamburg, Germany

We investigate the transport properties and non-equilibrium steady state phases of the dissipative ionic Hubbard model driven by an electric field. In the ionic Hubbard model, metallic behavior is enhanced by a competition of band insulating and Mott insulating behavior. The system is analyzed by means of the inhomogeneous dynamical mean-field theory (DMFT), using the iterated perturbation theory as impurity solver. The steady states of this model are accessed directly through the Keldysh contour formalism. We report results at half-filling for different interaction strengths, temperatures and geometries.

TT 19.67 Mon 15:00 P2-EG

Time propagation of systems with long range interaction in the framework of matrix product states — •Lars-Hendrik Frahm, Maximilian Hollstein, and Daniela Pfannkuche — I. Institut für Theoretische Physik, Universität Hamburg

The framework of matrix product states (MPS) has been seen to be more than just a compact technique to describe correlations in the density matrix renormalization group (DMRG) method. Among many other applications, MPS also turned out to allow for an efficient treatment of time-dependent systems. In this contribution, we benchmark the time-dependent MPS concept for systems with long range interaction (e.g. molecules). This type of system is especially challenging to approach since there is no fundamental law that guarantees a proper MPS representation (like there is for ground states in 1D local

systems). We discuss how to capture the necessary correlations with truncated MPS and how this truncation influences the time evolution after a quench. We compare our results to the time-dependent multi-reference configuration interaction singles (TDMRCIS) method, which is able to capture all correlations but only in a specific subspace of Hilbert space.

TT 19.68 Mon 15:00 P2-EG

Ultrafast dynamics of correlated fermions in lattice systems: Spectral properties — •Jan-Philip Joost, Niclas Schlünzen, and Michael Bonitz — CAU Kiel, Germany

The spectral properties of the infinite 1D Hubbard chain in the ground state can be described exactly by the Bethe ansatz [1]. However, for higher dimensional systems or the description of dynamical processes this spectral analysis becomes a challenging task. The nonequilibrium Green functions [2] (NEGF) approach grants easy access to the time-resolved spectral properties of extended and strongly correlated systems and is therefore well-suited to fill this gap [3]. Here, we present time-dependent and spatially resolved results for the spectral function and the dispersion relation of 1D and 2D systems in the ground state as well as for various nonequilibrium excitations. From a methodological point of view we compare different many body approaches, including the second Born, T-matrix and the third order approximation.

[1] F. H. L. Essler *et al.*, *The One-Dimensional Hubbard Model* (Cambridge University Press, 2005)
[2] K. Balzer and M. Bonitz, Lect. Notes Phys. **867** (2013)
[3] N. Schlünzen *et al.*, Phys. Rev. B **93**, 035107 (2016)

TT 19.69 Mon 15:00 P2-EG

The 1D Anderson model revisited: Low-frequency behavior of the optical conductivity — •Tim Breidenbach and Robin Steinigeweg — University Osnabrück

We study the low-frequency dependence of the optical conductivity $\mathrm{Re}\,\sigma(\omega)$ of the one-dimensional Anderson model, i.e., for non-interacting spin-less fermions in a random on-site potential. Using the method of exact diagonalization and dynamical quantum typicality, we calculate the real-time decay of the current autocorrelation function and obtain $\mathrm{Re}\,\sigma(\omega)$ by the Fourier transform of long-time data. We particularly variate the strength of disorder to determine low-frequency power laws at finite temperatures and in finite systems as well as the range of validity of Mott's law. Our results may shed light on corresponding studies in the many-body case, e.g., [1].

[1] R. Steinigeweg *et al.*, Phys. Rev. B **94**, 180401(R) (2016)

TT 19.70 Mon 15:00 P2-EG

Nonequilibrium dynamics of correlated fermions in lattice systems: A benchmark analysis of the nonequilibrium Green functions approach — •Niclas Schlünzen[1], Jan-Philip Joost[1], Fabian Heidrich-Meisner[2], and Michael Bonitz[1] — [1]CAU Kiel, Germany — [2]LMU München, Germany

The nonequilibrium dynamics of correlated fermions in lattice systems are of high current interest in the communities of both condensed matter and ultacold atoms. While there is a very fruitful progress in present experiments (e.g. Ref. [1]), the theoretical description constitutes a challenging task, especially in the regime of strong coupling and higher dimensions. Recently, two-dimensional quantum simulations of the expansion of fermions based on nonequilibrium Green functions[2] (NEGF) have been presented[3] that showed excellent agreement with the experiments. We present a benchmark analysis of the NEGF approach compared to results of the numerically accurate density matrix renormalization group (DMRG) method[4], which predominantly has been limited to one dimenional systems. The results indicate that NEGF can compete for weak to intermediate coupling strengths while being easily extendable to higher dimensions, larger system sizes and longer propagation times.

[1] U. Schneider *et al.*, Nat. Phys. **8**, 213 (2012)
[2] K. Balzer and M. Bonitz, Lect. Notes Phys. **867** (2013)
[3] N. Schlünzen, S. Hermanns, M. Bonitz, and C. Verdozzi, Phys. Rev. B **93**, 035107 (2016)
[4] N. Schlünzen *et al.*, submitted for publication (2016)

TT 20: Poster Session: Correlated Electrons 2

Time: Monday 15:00–19:00 Location: P2-OG1

TT 20.1 Mon 15:00 P2-OG1

Mott-Hubbard transition in the mass-imbalanced Hubbard model — •Marie-Therese Philipp, Markus Wallerberger, Patrik Gunacker, and Karsten Held — Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

The mass-imbalanced Hubbard model (HM) represents a continuous evolution from the Hubbard to the Falicov-Kimball model. We employ DMFT and study the paramagnetic metal-insulator transition (MIT). Our results indicate that the MIT rather resembles that of the HM as soon as a tiny hopping between the more localized fermions is switched on. Further due to the equalising power of the Kondo e ect, the MIT occurs simultaneously for both spin species, opposed to what is known for the multi-orbital HM.

TT 20.2 Mon 15:00 P2-OG1

LDA+DMFT approach to core-level X-ray spectroscopy for transition metal compound — •Atsushi Hariki[1], Takayuki Uozumi[2], and Jan Kuneš[1] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Department of Mathematical Sciences, Graduate School of Engineering, Osaka Prefecture University, Sakai, Osaka 599-8531, Japan

We perform systematic theoretical analysis of $2p$ core-level X-ray photoemission spectroscopy (XPS) of transition-metal compounds by means of the LDA+DMFT-based theoretical framework, which was recently developed [1,2]. In recent high-resolution and bulk-sensitive experiments, fine spectral features have become observed in the main-line (ML) structure of the $2p$ XPS. An account for these spectral features is essentially beyond the capability of theoretical models, such as the cluster model, conventionally employed in the analysis of $2p$ XPS. We reproduce the ML features by the new framework and show that these fine spectral features provide rich information on valence states including spin and orbital orderings.

[1] A. Hariki et al., J. Phys. Soc. Jpn. 82, 043710 (2013).
[2] A. Hariki et al., Eur. Phys. Lett. 114, 27003 (2016).

TT 20.3 Mon 15:00 P2-OG1

Systematic analysis of Lock-Crisp-West (LCW) back-folding — •Markus Dutschke[1], Michael Sekania[1,2], and Liviu Chioncel[1,3] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Andronikashvili Institute of Physics, Tamarashvili 6, 0177 Tbilisi, Georgia — [3]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

The LCW theorem provides a analytic transformation of the momentum distribution, obtained either by Compton profile or positron angular correlation measurements, into the electronic distribution in the irreducible part of the Brillouin zone. It is typically employed to identify Fermi surface sheets as discontinuities of the obtained data for the system under consideration. In practice, however, the measured or computed projected momentum distributions are of finite precision and limited in momentum range. These restrictions introduce artificial discontinuities in the LCW back-folded data, resulting in unphysical Fermi surface features. In our study we present a systematic analysis of different practical LCW implementations, which reduce artifacts of the transformation and increase accuracy. We present results for elemental bcc and fcc metals with already well known Fermi surfaces.

TT 20.4 Mon 15:00 P2-OG1

Characterization of the Mott-insulating phase in the one-dimensional fermionic Hubbard model — •Daniel Duarte, Daniela Pfannkuche, and Marta Prada — I. Institut für Theoretische Physik, Universität Hamburg

In general, many-body long range correlations after a localized quench show non-trivial behavior. We focus on the one dimensional Hubbard model in the Mott-insulating phase and we investigate the evolution of the characteristic long range correlations. The spatial dependence of the correlation functions on the interaction strength is investigated at low temperatures. Furthermore, the spatial-temporal spread of the

correlations after a sudden localized perturbation is calculated within a many-body description. Our analysis is based on a density matrix renormalization group approximation.

TT 20.5 Mon 15:00 P2-OG1

Field Control of Magnonic Heat Flow — •Benjamin Köhler and Wolfram Brenig — Institute for Theoretical Physics, Technische Universität Braunschweig, Germany

Insulating quantum magnets allow for genuine spin transport phenomena without carrier dynamics. Controlling such transport by means of external fields is vital for potential device design. Here we study thermal conductivity of a two dimensional square lattice spin-1/2 Heisenberg antiferromagnet in the presence of either external magnetic or electric fields. These fields are used to manipulated the heat flow, due to spin canting for the former and due to coupling to an additional Dzyaloshinsky-Moriya interaction for the latter. Using nonlinear spin wave theory and a Kubo approach we evaluate the thermal conductivity taking into account current relaxation by extrinsic mechanisms, as well as intrinsic magnon decay for finite magnetic fields. Semi-quantitative estimates for attainable variations of the heat conductivity in realistic materials will be presented as a function of the temperature and the external fields.

TT 20.6 Mon 15:00 P2-OG1

Stochastic analytic continuation of Quantum Monte Carlo data — •Niklas Casper and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

Analytical continuation of imaginary time data from Quantum Monte Carlo methods is a notoriously complicated numerical task which is mathematically ill posed. Recently, stochastic analytic continuation (SAC) methods, which map the inversion from imaginary time to real frequencies onto a classical field theory at a fictitious temperature, have been introduced as a potential superset of conventional maximum entropy methods (MEM). We provide a complementary analysis of spectra obtained from SAC as well as MEM, resulting from various test models, as well the dynamic structure factor of a prototypical spin chain. We analyze the thermodynamics of the SAC considering various proposals for the choice of an optimal fictitious temperature. Moreover, we implement an auxiliary parallel Wang-Landau algorithm to provide for an unbiased determination of the spectrum, using the prior probability.

TT 20.7 Mon 15:00 P2-OG1

Reduced Density-Matrix Functionals from Green's Functions — •Heike Eisenlohr[1], Ebad Kamil[1], Robert Schade[2], and Peter Blöchl[2] — [1]Institute for Theoretical Physics, University of Goettingen, Goettingen, Germany — [2]Institute for Theoretical Physics, Clausthal University of Technology, Clausthal, Germany

A new method for the electronic structure calculations of strongly correlated materials is explored. The long-term goal is the efficient simulation of such materials in the context of first-principles calculations. The method rests on an exact theorem, which expresses the one-particle reduced density-matrix functional by many-particle Green's functions via the Luttinger-Ward functional [1]. This theorem makes contact between ground state approaches such as reduced density matrix functional theory (rDMFT) and Feynman diagrams and even non-perturbative many-particle methods. The theorem suggests new approximate methods for the construction of density matrix functionals, namely to first establish an empirical Green's function as a direct function of the reduced density matrix, and secondly to evaluate the energy for this Green's function with many-particle methods. We present results based on a diagrammatic expansion and discuss difficulties and successes on the example of the Hubbard dimer.

This work is supported by the Deutsche Forschungsgemeinschaft via FOR1346 through project P9.

[1] P. E. Blöchl et al., Phys. Rev. B 88, 205139 (2013).

TT 20.8 Mon 15:00 P2-OG1

From local to non-local correlations: the Dual Boson perspective — •Arthur Huber — Universitaet Hamburg

Extended dynamical mean-field theory (EDMFT) is insufficient to describe non-local effects in strongly correlated systems, since corrections to the mean-field solution are generally large. We present an efficient scheme for the construction of diagrammatic extensions of EDMFT that avoids usual double counting problem by using an exact change of variables (the dual boson formalism) to distinguish the correlations included in the mean-field solution and those beyond. With a computational efficiency comparable to EDMFT+GW approach, our scheme significantly improves on the charge order transition phase boundary in the extended Hubbard model.

TT 20.9 Mon 15:00 P2-OG1

Susceptibility calculations using a multi-orbital general CT-QMC solver for DMFT — •Julian Musshoff[1,2], Amin Kiani[1], and Eva Pavarini[1] — [1]Forschungszentrum Juelich GmbH, Institute for Advanced Simulation, 52425 Juelich, Germany — [2]Institute for Theory of Statistical Physics RWTH Aachen University, 52074 Aachen, Germany

Susceptibilities describe the response of a system to an external perturbation, and are therefore essential to compare theoretical calculations with experiments. We use a general continuous-time quantum Monte Carlo solver [1] for dynamical mean-field theory to calculate generalized local susceptibilities. Our general solver allows us to study multi-orbital correlated systems of any symmetry. We calculate the lattice susceptibilities using the Bethe-Salpeter equation. On the poster we show magnetic susceptibility results for a representative multi-orbital system, $KCuF_3$.

[1] A. Flesch, E. Gorelov, E. Koch, E. Pavarini, *Phys. Rev. B 87*, 195141

TT 20.10 Mon 15:00 P2-OG1

Luttinger theorem in strongly correlated multi-orbital systems — •Johannes Mitscherling[1,2] and Eva Pavarini[1] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

The Luttinger theorem stating that the volume enclosed by the Fermi surface is entirely determined by the total particle number was originally derived for a Fermi liquid in the zero temperature limit. We discuss the possible extension of the theorem for certain classes of strongly correlated systems outside the Fermi-liquid regime.

Similarly to Luttinger's sum rule, we present a sum rule for correlated multi-orbital systems at finite temperature. We identify an exact relation between the Fermi volume of a given band index and its occupation. This relation involves additional contributions which come into play in this generalized setting while they vanish for a Fermi liquid in the zero temperature limit. The study of these contributions enables us to identify conditions under which the Luttinger theorem is valid beyond its traditional scope.

As a first application, we apply the extended Luttinger sum rule to the two-site Hubbard model. As a second step, the extended Luttinger theorem is used to study the temperature evolution of the three Fermi sheets of Sr_2RuO_4.

TT 20.11 Mon 15:00 P2-OG1

Screened Coulomb interaction for strongly correlated molecular crystals — •Michael M. E. Baumgärtel and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

For strongly correlated molecular crystals we determine screened Coulomb Hubbard-parameters. The unscreened Coulomb interaction of correlated molecular orbitals (MOs) can directly be obtained from Hartree-integrals. This interaction is screened by the electrons in the uncorrelated MOs as these are polarized. We compute the screening due to the self-consistent electric fields arising from the induced distributed dipoles. To treat the polarized crystal, we develop an optimized Ewald summation of the Fourier-transformed dipole-dipole interaction. Employed on a Brillouin zone grid our method yields the screened inter-molecular Coulomb interaction for any charging pattern of the correlated MOs. The optimization of the convergence and performance of our method is demonstrated.

We present the screened Coulomb interaction e.g. for Fullerene crystals and discuss the accuracy and reliability of the results. While in the past only approximations of MOs as a single point-dipole where feasible, we discuss the effect of spacially extended MOs: For example for Fullerenes we approach the limit of point-dipoles by virtually shrinking the Fullerene radius and we determine the renormalization of the polarizabilities due to distribution of the MOs.

TT 20.12 Mon 15:00 P2-OG1

Scaling Behavior of the Compton Profile of Alkali Metal Elements — •Michael Sekania[1,2], Wilhelm Hans Appelt[3,4], Diana Benea[5], Hubert Ebert[6], Dieter Vollhardt[1], and Liviu

Chioncel[1,4] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Andronikashvili Institute of Physics, 0177 Tbilisi, Georgia — [3]Theoretical Physics II, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [4]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [5]Faculty of Physics, Babes-Bolyai University, Ro-400084 Cluj-Napoca, Romania — [6]Department of Chemistry, University Munich, D-81377 München, Germany

The contribution of the valence electrons to the Compton profiles of the alkali metals is calculated using density functional theory. We show that the Compton profiles can be modeled by a $q-$Gaussian distribution, which is characterized by an anisotropic, element dependent parameter q. Thereby we derive an unexpected scaling behavior of the Compton profiles of all alkali metals.

TT 20.13 Mon 15:00 P2-OG1

Exact Diagonalization study of large Hubbard clusters — •Michael Danilov[1], Sergei Iskakov[2], Malte Harland[1], and Alexander Lichtenstein[1] — [1]I. Institut für Theoretische Physik Jungiusstrasse 9, 20355 Hamburg, Germany — [2]Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA

Using efficient exact diagonalization scheme, we studied electronic structure of 4x4 doped Hubbard cluster with realistic hopping parameters including next nearest neighbour hopping t′ = -0.3t, which is optimal for superconducting cuprates. The Green's function and abnormally large density of states near Fermi level are analysed as function of doping and strength of local Coulomb interactions.

In order to compare the spectrum of the 16-site cluster against small 2x2 plaquette, where the ground state is 6-fold degenerate for special values of Coulomb interactions and chemical potential (Phys. Rev. B 94 (2016) 125133), we scale the hopping between the 4 plaquettes constituting the cluster with auxiliary parameter α.

We examined the degeneracy of low-energy spectra as function of α and local Coulomb interaction U and visualised the ground state wavefunction. Our current standpoint is that the optimal Coulomb interaction is close to U=10t, versus U=6t for degenerate ground state of isolated plaquette. We discuss the relevance of degenerate low-energy spectra with regard to possible mechanism of the high-temperature superconductivity.

TT 20.14 Mon 15:00 P2-OG1

Quantum-Many-Body Intermetallics: Phase Stability of Fe 3 Al and Small-Gap Formation in Fe 2 VAl — •Oleg Kristanovski — I. Institut für Theoretische Physik Jungiusstrasse 9, 20355 Hamburg, Germany

Various intermetallic compounds harbor subtle electronic correlation effects. To elucidate this fact for the Fe-Al system, we perform a realistic many-body investigation based on the combination of density functional theory with dynamical mean-field theory in a charge self-consistent manner. A better characterization and understanding of the phase stability of bcc-based D0 3 -Fe 3 Al through an improved description of the correlated charge density and the magnetic-energy is achevied. Upon replacement of one Fe sublattice by V, the Heusler compound Fe 2 VAl is realized, known to display bad-metal behavior and increased specific heat. We here document a charge-gap opening at low tem- peratures in line with previous experimental work. The gap structure does not match conventional band theory and is reminiscent of (pseudo)gap charateristics in correlated oxides.

TT 20.15 Mon 15:00 P2-OG1

Reservoir-induced Collapse and Revival of Photon BEC Oscillations — •Bastian Havers, Tim Lappe, and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

A true photon Bose-Einstein condensate (BEC) was first realized in 2010 [1] by filling a dense photon gas into a dye-filled, optical microcavity by means of a laser and subsequently thermalizing it at room temperature. Most recently, the dynamics is being investigated by means of Josephson oscillations of the photon BEC in double-well potential traps. It is characterized by a collapse and revival of Josephson oscillations. We develop the theory for the photon BEC dynamics, coupled to the dye. The ensemble of dye molecules is described as a structured, dissipative bath of three-level systems, involving three different processes, photon absorption with absorption rate $1/\tau_a$, dark transitions, and photon re-emission with emission rate $1/\tau_e$. The BEC dynamics is treated on the Gross-Pitaevskii level in a two-mode approximation for the BECs in the two potential wells [2].

[1] J. Klaers, J. Schmitt, F. Vewinger, and M. Weitz, Nature **468**, 545 (2010).
[2] A. Smerzi, S. Fantoni, S. Giovanazzi, and S. R. Shenoy, Phys. Rev. Lett. **79**, 4950 (1997)

TT 20.16 Mon 15:00 P2-OG1

Higher-order local and non-local correlations for 1D strongly interacting Bose gas — EJKP Nandani[1,2,3], •Rudolf A Römer[4], Shina Tan[5,6], and Xi-Wen Guan[1,7] — [1]Wuhan Institute of Physics and Mathematics, CAS, Wuhan 430071, China — [2]Chinese Academy of Sciences, Beijing, China — [3]University of Ruhuna, Matara, Sri Lanka — [4]University of Warwick, Coventry CV4 7AL, UK — [5]Georgia Institute of Technology, Atlanta, GA, USA — [6]Center for Cold Atom Physics, Wuhan, China — [7]Australian National University, Canberra ACT 0200, AUS

The correlation function is an important quantity in the physics of ultracold quantum gases because it provides information about the quantum many-body wave function beyond the simple density profile. In this paper we first study the M-body local correlation functions of the one-dimensional (1D) strongly repulsive Bose gas within the Lieb-Liniger model using the analytical method proposed by Gangardt and Shlyapnikov (2003 Phys. Rev. Lett. 90 010401; 2003 New J. Phys. 5 79). In the strong repulsion regime the 1D Bose gas at low temperatures is equivalent to a gas of ideal particles obeying the non-mutual generalized exclusion statistics with a statistical parameter $\alpha = 1 - 2/\gamma$. Here γ is the dimensionless interaction strength within the Lieb-Liniger model. We rigorously prove that such a statistical parameter solely determines the sub-leading order contribution to the M-body local correlation function of the gas at strong but finite interaction strengths. We explicitly calculate the correlation functions at zero, low, and intermediate temperatures.

TT 20.17 Mon 15:00 P2-OG1

Spin dynamics in classical XXZ chains with disorder — •Tim Dierker and Robin Steinigeweg — University Osnabrück

The transport of magnetization is analyzed for the classical XXZ spin chain with a random magnetic field. In order to do so, the Hamiltonian equations of motion are solved numerically for initial states realizing harmonic-like magnetization profiles with small amplitudes and with random phases. Without disorder, the resulting dynamics are observed to be diffusve in a hydrodynamic regime starting at comparativley small times and wave lengths [1]. The influence of disorder on these dynamics is studied in the entire range from weak to strong disorders.

[1] R. Steinigeweg, Europhysics Letters 97, 67001 (2012)

TT 20.18 Mon 15:00 P2-OG1

Numerical Study of the Kitaev-Heisenberg Chain — •Cliò Efthimia Agrapidis[1,2], Jeroen van den Brink[1,2], and Satoshi Nishimoto[1,2] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany — [2]Department of Physics, Technical University Dresden, 01069 Dresden, Germany

In recent years, because of the emergence of candidate materials and the interest in the spin liquid state realization, there has been a growing number of studies on the Kitaev model, at first, and on the Kitaev-Heisenberg (KH) after. Adding the Heisenberg-type interaction to the initial, exactly integrable, model is necessary and inevitable for any realistic description. Nevertheless, the vast majority of these studies is focused on 2-dimensional lattices (honeycomb, triangular), while research on the KH chain is lacking.

Motivated by this, we study the KH chain using the exact diagonalization and the density matrix renormalization group techniques. We present the phase diagram as a function of an angle parameter ϕ, setting the Heisenberg interaction to $\cos\phi$ and the Kitaev one to $\sin\phi$. We identify five different possible phases; namely, Heisenberg, incommensurate, ferromagnetic, XY and Néel phases, by calculating total spin, central charge, static structure factor, and the Néel and XY order parameters. Moreover, we investigate specific features of the dynamical structure factor in each phase. In addition, we present some of the above calculations in the presence of an applied magnetic field.

TT 20.19 Mon 15:00 P2-OG1

Topological properties of classical spin spirals from an exact mapping to free fermions — •Jan Attig and Simon Trebst — University of Cologne

In classical magnets coplanar spin spirals often arise in the presence of competing interactions which suppress more conventional types of magnetic order. Here we demonstrate that the physics of these coplanar spin spirals can be understood from an exact mapping of the classical Heisenberg model on a geometrically frustrated lattice to a free-fermion model on a closely related "squared" lattice. This one-to-one correspondence not only allows to make a connection between the Fermi surface of the free fermion model and the manifold of degenerate spiral states, but also allows to discuss topological phenomena of the free-fermion band structure in the corresponding classical magnet.

TT 20.20 Mon 15:00 P2-OG1

Competing spin textures in j=1/2 Mott insulators on the triangular lattice — •Tilman Disselkamp and Simon Trebst — University of Cologne

Similar to their well-studied electronic counterparts, quantum magnets exhibit a wealth of novel phenomena in the presence of strong spin-orbit coupling. Of particular interest are Kitaev materials, spin-orbit entangled j=1/2 Mott insulators where topology plays a key role in the formation of magnetic order – either in the emergence of spin liquid physics or, of interest here, the formation of non-trivial spin textures. Specifically, we consider j=1/2 Mott insulators in triangular lattice geometries, relevant e.g. to the sister compounds $Ba_3IrTi_2O_9$ and $Ba_3TiIr_2O_9$ for which we study the interplay of geometric frustration and spin-orbit coupling. The latter gives rise to Kitaev or Dzialoshinskii-Moriya interactions that stabilize a Z_2 vortex crystal or a skyrmion crystal, respectively. Using classical Monte Carlo simulations, we map out the stability and interplay of these spin textures in a magnetic field at zero and finite temperatures.

TT 20.21 Mon 15:00 P2-OG1

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 certain time to be formed. The influence of a 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 how the screening and collective modes are build up.

[1] K. Morawetz, Phys. Rev. B 90 (2014) 075303
[2] K. Morawetz, Phys. Rev. E 66 (2002) 022103
[3] K. Morawetz, M. Bonitz, V. G. Morozov, G. Röpke, D. Kremp, Phys. Rev. E 63 (2001) 20102
[4] K. Morawetz, V. Spicka, P. Lipavský: Phys. Lett. A 246 (1998) 311

TT 21: Focus Session: Nematicity, Magnetism and Superconductivity in FeSe and Related Compounds

Iron based superconductors form the largest family of unconventional superconductors known to us. Among these, the FeSe systems present a curious phenomenology: almost all members related to this family exhibit $T_c \sim$ 35-45 K, and even reaching 60-70 K in the case of single unit cell thick FeSe grown on $SrTiO_3$ (STO). Furthermore, bulk FeSe demonstrates a peculiar phase diagram with variety of transitions including nematic (structural), magnetic and the superconducting one. The nature of the phase competition between superconductivity and other phases is qualitatively different from what is seen in other iron based systems and likely tied to the strong mixing between s- and d-wave Cooper pairing. The aim of this focus session is to bring together the leading experimental and theoretical experts, and thus to directly address some of the most pressing controversies in this field.

Organization: Ilya Eremin, Universität Bochum; Jörg Schmalian, KIT

Time: Tuesday 9:30–12:15 Location: HSZ 03

Invited Talk TT 21.1 Tue 9:30 HSZ 03

BCS-BEC Crossover, Preformed Pairs and Highly Spin-Polarized Superconducting Phase in FeSe — •Yuji Matsuda — Kyoto University, Kyoto, Japan

There is growing evidence that superconducting semimetal FeSe (T_c=8K) is deep in the crossover regime between weak coupling Bardeen-Cooper-Schrieffer (BCS) and strong-coupling Bose-Einstein-condensate (BEC) limits. Therefore FeSe offers a unique and fascinating platform to study the crossover physics. Here we discuss several unique features which may provide new insights into fundamental aspects of the crossover. First is the observation of giant superconducting fluctuations by far exceeding the standard Gaussian theory and a possible pseugogap formation above T_c. Second is the electronic structure. FeSe is a compensated semimetal, and hence it is essentially multiband superconductor, which makes the crossover physics in FeSe distinguished from that in ultracold atomic gases. Third concerns the fate of the superfluid when the spin populations are strongly imbalanced. In FeSe in the crossover regime, the Zeeman effect is especially effective in shrinking the Fermi volume associated with the spin minority. We show the emergence of a distinct field-induced superconducting phase, which has an unprecedentedly large spin-imbalance.

Invited Talk TT 21.2 Tue 10:00 HSZ 03

Discovery of Orbital-Selective Cooper Pairing in FeSe — •J. C. Séamus Davis[1], Peter Sprau[2], Andrey Kostin[2], Andreas Kreisel[3], Anna Böhmer[4], Paul Canfield[4], S. Mukherjee[5], Peter Hirschfeld[6], and Brian Andersen[7] — [1]Department of Physics, Cornell University, Ithaca, NY 14853, USA. — [2]Brookhaven National Laboratory, Upton, NY 11973, USA. — [3]Universität Leipzig, D-04103 Leipzig, Germany — [4]Ames Laboratory, U.S. Department of Energy, Ames, IA 50011, USA — [5]Binghamton University - SUNY, Binghamton, USA. — [6]University of Florida, Gainesville, Florida32611, USA — [7]University of Copenhagen, DK 2100 Copenhagen, Denmark

FeSe is the focus of intense research interest as the basis for achieving the highest critical temperatures of any iron-based superconductor. However, its Cooper pairing mechanism has not been determined because an accurate knowledge of the momentum-space structure of superconducting energy gaps on the different electron-bands does not exist. Here we use Bogoliubov quasiparticle interference (BQPI) imaging to determine the coherent Fermi surface geometry of multiple bands, and to measure their superconducting energy gaps. We show directly that both gaps are extremely anisotropic but nodeless, and of opposite sign. This complex configuration of energy gaps which was unanticipated by existing pairing theories for FeSe, reveals a unique form of superconductivity based on orbital-selective Cooper pairing of electrons from the dyz orbitals of iron atoms.

Invited Talk TT 21.3 Tue 10:30 HSZ 03

Frustrated Magnetism and Electron-Electron Interactions in FeSe — •Roser Valenti — Goethe University Frankfurt, Germany

The temperature-pressure phase diagram of bulk FeSe continues to fascinate a large fraction of researchers working on unconventional superconductivity. In this talk, we will discuss this phase diagram from a first principles prespective. We will show that the magnetic interactions in chalcogenides, as opposed to pnictides, demonstrate un-

usual frustration, which suppresses magnetic, but not nematic order, favors orbital order in the nematic phase and can naturally explain the nonmonotonic pressure dependence of the superconducting critical temperature. Furthermore we will argue on the importance of electron-electron interactions in FeSe and compare our results based on a combined first principles with many-body methods study with available recent experimental results.

15 min. break.

Invited Talk TT 21.4 Tue 11:15 HSZ 03

Orbital-Selective Pairing and Gap Structures of Iron-Based Superconductors — •Brian Andersen — Juliane Maries Vej 30, 2100 Copenhagen, Denmark

Recent experiments in the superconducting phase of iron-based superconductors have mapped out the detailed momentum dependence of the superconducting gap structure. We discuss the influence on spin-fluctuation pairing theory of orbital selective strong correlation effects in Fe-based superconductors, particularly Fe chalcogenide systems. We propose that a key ingredient for an improved itinerant pairing theory is orbital selectivity, i.e. incorporating less coherent quasiparticles occupying specific orbital states into the pairing theory. This modifies the usual spin-fluctuation pairing via suppression of pair scattering processes involving those incoherent states and results in orbital selective Cooper pairing of electrons in the remaining states. We show that this paradigm yields remarkably good agreement with the experimentally observed anisotropic gap structures in both bulk and monolayer FeSe, as well as LiFeAs, indicating that orbital selective Cooper pairing plays a key role in the more strongly correlated iron-based superconductors.

Invited Talk TT 21.5 Tue 11:45 HSZ 03

New Experimental Results Concerning the Nematic State in Fe-based Superconductors — •Christoph Meingast — Institute for Solid State Physics, Karlsruhe Institute of Technology, Germany.

The nature of the nematic state in FeSe and Ba-122 systems is studied using a variety of experimental probes. In particular, we use a new technique, in which a considerable uniaxial strain is applied to the crystals by glueing them to a substrate with a large anisotropic thermal expansion, to measure the in-plane anisotropy of the uniform magnetic susceptibility and the resistivity under large strains [1]. We discuss the scaling of these quantities for both Ba-122 and FeSe. Further, we study the shear-modulus response of the C4-reentrant phase in Na - doped Ba-122 using a three-point bending technique. Surprisingly, we still find a sizeable nematic susceptibility in this phase, which further increases upon entering the superconducting state, in strong contrast to the behavior of optimally doped crystals. This is likely related to the strong competition between superconductivity with the double-Q state, as our previous studies have shown [2,3]. Finally, we study the coupling between nematicity and superconductivity of FeSe crystals using thermal expansion, magnetostriction and heat capacity. Surprisingly, the orthorhombic distortion is enhanced by superconductivity in S-substituted FeSe [4]. Heat capacity data point to a nodal superconducting gap structure.

[1] M. He et al., arXiv:1610.05575.
[2] A. E. Boehmer et al., Nat. Commun. 6, 7611 (2015).
[3] L. Wang et al., PRB 93, 014514 (2016)
[4] L. Wang et al., physica status solidi (b) 1-6 (2016), 10.1002/pssb.201600153.

TT 22: Transport: Quantum Coherence and Quantum Information Systems - Theory (jointly with MA, HL)

Time: Tuesday 9:30–13:15 Location: HSZ 103

TT 22.1 Tue 9:30 HSZ 103

Adiabatic Quantum Simulations with Superconducting Qubits — •Nikolaj Moll, Panagiotis Barkoutsos, Daniel Egger, Stefan Filipp, Andreas Fuhrer, Marc Ganzhorn, Andreas Kuhlmann, Peter Müller, Marco Roth, Peter Staar, and Ivano Tavernelli — IBM Research – Zurich, Säumerstrasse 4, CH-8803 Rüschlikon, Switzerland

Quantum computing technology is improving fast and quantum computers with approximately 100 qubits appear feasible in the not so distant future. The quest for systems which profit of exponential speed-up and cannot be calculated on classical computers has recently triggered a lot of attention. Fermionic quantum systems, such as quantum chemistry or the Fermi-Hubbard model, are among the best candidates for exploiting the exponential speed-up. Such a quantum system can be implemented on a quantum computer based on superconducting qubits. However, the controlled realization of different types of interactions between qubits without compromising their coherence is essential. A coupling method between fixed-frequency transmon qubits can be achieved with the frequency modulation of an auxiliary capacitively coupled quantum bus. An adiabatic protocol for the Hydrogen molecule can be implemented on such a coupled qubit system.

TT 22.2 Tue 9:45 HSZ 103

Tunable, Flexible and Efficient Optimization of Control Pulses for Superconducting Qubits, part I - Theory — •Shai Machnes[1,2], Elie Assémat[1], David Tannor[2], and Frank Wilhelm[1] — [1]Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Weizmann Institute of Science, 76100 Rehovot

Quantum computation places very stringent demands on gate fidelities, and experimental implementations require both the controls and the resultant dynamics to conform to hardware-specific ansatzes and constraints. Superconducting qubits present the additional requirement that pulses have simple parametrizations, so they can be further calibrated in the experiment, to compensate for uncertainties in system characterization. We present a novel, conceptually simple and easy-to-implement gradient-based optimal control algorithm, GOAT [1], which satisfies all the above requirements.

In part II we shall demonstrate the algorithm's capabilities, by using GOAT to optimize fast high-accuracy pulses for two leading superconducting qubits architectures - Xmons and IBM's flux-tunable couplers.

[1] S. Machnes, D.J. Tannor, F.K. Wilhelm and E. Assémat, ArXiv 1507.04261 (2015)

TT 22.3 Tue 10:00 HSZ 103

Tunable, Flexible and Efficient Optimization of Control Pulses for Superconducting Qubits, part II: Applications — Shai Machnes[1,2], •Elie Assemat[1], David Tannor[2], and Frank Wilhelm[1] — [1]Saarland University, Saarbrücken, Germany — [2]Weizmann Institute of Science, Rehovot, Israel

In part I, we presented the theoretic foundations of the GOAT algorithm [1] for the optimal control of quantum systems. Here in part II, we focus on several applications of GOAT to superconducting qubits architecture. First, we consider a control-Z gate on Xmons [2] qubits with an Erf parametrization of the optimal pulse. We show that a fast and accurate gate can be obtained with only 16 parameters, as compared to hundreds of parameters required in other algorithms. We present numerical evidences that such parametrization should allow an efficient in-situ calibration of the pulse. Next, we consider the flux-tunable coupler by IBM [3]. We show optimization can be carried out in a more realistic model of the system than was employed in the original study, which is expected to further simplify the calibration process. Moreover, GOAT reduced the complexity of the optimal pulse to only 6 Fourier components, composed with analytic wrappers.

[1] S. Machnes et al., ArXiv 1507.04261v1 (2015)
[2] R. Barends et al., Phys. Rev. Lett. 100, 080502 (2013)
[3] D. C. McKay et al., ArXiv 1604.0307v2 (2016)

TT 22.4 Tue 10:15 HSZ 103

Symmetry Benchmarking of Quantum Algorithms — •Tobias Chasseur Chasseur[1], Felix Motzoi[1,2], Michael Kaicher[1], Pierre-Luc Dallaire-Demers[1], and Frank Wilhelm[1] — [1]Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark

Scalable and robust benchmarking of quantum gates is essential on the path to a useful quantum computer, as current candidates such as

superconducting qubit systems are set to leave the few qubit regime in the near future. Randomized Benchmarking and related approaches provide solutions for specific gates such as the Clifford group or a limited number of qubits; however a tool for benchmarking arbitrary gates without exponential scaling in the number of qubits seems prohibited by the inherent power of quantum computation. In this work we present a symmetry benchmarking protocol to estimate the implementation fidelity of specific algorithms with polynomial scaling. The proposed protocol relies on unitary 1-designs on the eigenspaces of algorithm-specific preserved quantities, as well as sequence structures similar to Randomized Benchmarking. It benchmarks the symmetry preservation of the implementation as an indicator for the overall fidelity. We demonstrate the protocol for the specific example of algorithms consisting of number preserving gates.

TT 22.5 Tue 10:30 HSZ 103

Implementation of Quantum Stochastic Walks — •Peter Schuhmacher[1], Luke Govia[2], Bruno Taketani[1], and Frank Wilhelm[1] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Department of Physics, McGill University, Montreal, Quebec, Canada

Quantum walks are one of the most prominent frameworks in which to design and think about quantum algorithms. Both the continuous- and discrete-time versions have been shown to provide speed-up over classical information processing tasks, and can be regarded as universal quantum computers. Classical (probabilistic) and quantum unitary random walks yield different distributions due to interference effects. Combining the two, stochastic quantum walks (QSW) can be defined in an axiomatic manner to include unitary and non-unitary effects, and include both classical and quantum walks as limiting cases. While a general purpose quantum computer is still far over the horizon, intermediary technologies have been emerging with the promise to breach classical limitations. Within these, artificial intelligence is one exciting field where the use of quantum physics can lead to important improvements. Here, we focus on the physical realizability of both kinds of quantum stochastic walks (continuous-time and discrete-time).

TT 22.6 Tue 10:45 HSZ 103

Normal metal traps for superconducting qubits — •Roman-Pascal Riwar[1,2], Amin Hosseinkhani[1,3], Luke D. Burkart[2], Yvonne Y. Gao[2], Robert J. Schoelkopf[2], Leonid I. Glazman[2], and Gianluigi Catelani[1] — [1]Forschungszentrum Jülich, Germany — [2]Yale University, USA — [3]RWTH Aachen University, Germany

The coherence time of superconducting qubits is intrinsically limited by the presence of quasiparticles. While it is difficult to prevent the generation of quasiparticles, keeping them away from active elements of the qubit provides a viable way of improving the device performance. We develop theoretically and validate experimentally a model for the effect of a single small trap on the dynamics of the excess quasiparticles injected in a transmon-type qubit. By means of this model, we show that for small traps, increasing the size shortens the evacuation time of quasiparticles from the transmon. We further identify a characteristic trap size above which the evacuation time saturates to the diffusion time of the quasiparticles. In the diffusion limit, the geometry of the qubit and the trap become relevant. We compute the optimal trap number and placement for several realistic geometries. Finally, our estimates show that the dissipation introduced by the presence of normal metal traps is well below the losses observed in the transmon.

TT 22.7 Tue 11:00 HSZ 103

Proximity Effect in Normal-Metal Quasiparticle Traps — •Amin Hosseinkhani[1,2] and Ginaluigi Catelani[1] — [1]Peter Grunberg Institut (PGI-2), Forschungszentrum Jülich, Jülich, Germany — [2]JARA-Institute for Quantum Information, RWTH Aachen University, Aachen, Germany

In many superconducting devices, including qubits, quasiparticle excitations are detrimental. A normal metal (N) in contact with a superconductor (S) can trap these excitations. However, the contact between N and S modifies the properties of both materials, a phenomenon known as proximity effect which has drawn attention since the '60s. Despite this long history, we find new analytical results for the density of states, which shows a square root threshold behavior at the minigap energy. In superconducting qubits, the trap must be placed far enough from a Josephson junction in order not to harm the qubit coherence. To estimate the minimum trap-junction separation, we study how the density of states in the superconductor depends on the distance from the trap. For high interface resistance between N and S, a separation of several (5-7) coherence lengths is sufficient.

15 min. break.

TT 22.8 Tue 11:30 HSZ 103

Generating Entangled Quantum Microwaves in a Josephson-Photonics Device — •Simon Dambach, Björn Kubala, and Joachim Ankerhold — Institute for Complex Quantum Systems, Ulm University, Ulm, Germany

The realization of efficient sources for entangled microwave photons is of paramount importance for many promising applications of quantum technology. In this talk, we demonstrate that Josephson-photonics devices are logical candidates for this task since they allow to create a broad range of different bi- and multipartite entangled states in a surprisingly simple way [1].

In a Josephson-photonics device, a Cooper pair tunneling across a dc voltage-biased Josephson junction simultaneously creates photons in several series-connected microwave cavities. The interplay of this multiphoton creation process and subsequent individual photon leakage from the cavities leads to a stationary state with complex entanglement properties. Sophisticated pulse-shaping schemes as required in conventional circuit-QED architectures are thus not necessary here. Varying experimental parameters in situ or by construction then allows to access the rich wealth of entangled states differing, e.g., in the number of entangled parties or the dimension of state space. Such devices, besides their promising potential to act as a highly versatile source of entangled quantum microwaves, may be also an excellent playground for the abstract branch of quantum information theory to test entanglement criteria on naturally existing quantum states.
[1] S. Dambach, B. Kubala, and J. Ankerhold, arXiv:1609.08990

TT 22.9 Tue 11:45 HSZ 103

Theory of mode locking in pulsed semiconductor quantum dots — •Wouter Beugeling, Götz S. Uhrig, and Frithjof B. Anders — Lehrstuhl für Theoretische Physik 1/2, TU Dortmund, Dortmund, Germany

Electron spins in semiconductor quantum dots appear unsuitable for quantum computing at first sight, due to their fast decoherence caused by hyperfine interactions to the nuclear spins in the substrate. However, the coherence time is dramatically increased by periodic optical pulsing. The underlying mechanism is known as mode locking: Oscillation frequencies incommensurate with the pulse repetition rate are suppressed, and only resonant contributions remain. Because the resonant frequencies are set by the pulse repetition rate only, the system becomes effectively immune to perturbations induced by the hyperfine interactions and by variations between the individual quantum dots in an ensemble.

In this presentation, we explore the mechanism of mode locking with a combination of analytical and numerical methods. Exploiting the fact that the hyperfine interaction is small compared to the external magnetic field, we calculate the dynamics perturbatively. The resulting frequency distributions show clear signs of mode locking. We study the positions of the resonant frequencies and the rate at which mode locking sets in, and compare the results to other theoretical and experimental studies. We also discuss the influence of the hyperfine coupling strength, of the Zeeman effect of the nuclear spins, and of the pulse shape and detuning.

TT 22.10 Tue 12:00 HSZ 103

Higher Order Spin Correlation in Semi-Conductor Quantum Dots — •Nina Fröhling and Frithjof Anders — Technische Universität Dortmund, Deutschland

We study higher order auto-correlation functions of electron spin decay in an isolated semi-conductor quantum dot described by the central spin model. The electronic central spin is coupled to a bath of nuclear spins via hyperfine interaction, which dominates the short time regime. Via quantum measurement theory we show that the experiment by Bechtold et al. (Phys. Rev. Lett. 117. 027402, 2016) can be described as a fourth order auto-correlation function. We compare our results obtained from a semiclassical approach, exact diagonalization and a Lanczos algorithm to the experimental results. In order to explain the observed long time dynamics in the forth order autocorrelation the nuclear Zeeman splitting and the strain induced anisotropic quadrupolar moment of the nuclei must be included.

TT 22.11 Tue 12:15 HSZ 103

Non-equilibrium nuclear spin distributions in a periodically pulsed quantum dot — •Natalie Jäschke and Frithjof Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische

Physik II, 44227 Dortmund

In pump-probe experiments single electron charged semiconductor quantum dots are subjected to periodic optical excitations. This mechanism generates electron and nuclear spin polarization. In the short time regime the decoherence of the electron spin polarization is governed by the hyperfine interaction with the nuclear spins. We aim for a theory that combines the effect of the periodic laser pump pulses and the nuclear spin bath on the electron spin polarization. Since the laser pulses occur on the shortest time scale of the system, and the electronic decay times are small compared to those of the nuclear spin bath, we treat the laser pumping quantum-mechanically using a Lindblad approach and keep the nuclear spins as frozen during that time. Then a classical simulation of the Overhauser field bridges the time until the next laser pulse. On the one hand we analyze the time dependence of the electron spin dynamics and on the other hand present data for the non-equilibrium steady state spectral distributions of the Overhauser field for the long time limit. For the electron spin dynamics a revival effect right before the next pulse is observed. The Overhauser field shows mode locking effects in the component parallel to the external magnetic field.

TT 22.12 Tue 12:30 HSZ 103

Detection of coherent oscillations in proximitized quantum dot spin valves — Philipp Stegmann, Jürgen König, and •Stephan Weiss — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

Spin coherent oscillations in a proximitized quantum dot spin valve are resolved by means of full counting statistics of electrons [1]. Especially, generalized factorial cumulants [2,3] of the electronic distribution function are suitable for the detection of the transition between different spin states in the system. We furthermore study the influence of a tunnel coupled superconductor. Due to the presence of Andreev reflections, coherent oscillations between different spin states are modified, the Larmor frequency is renormalized. We explore that general factorial cumulants are able to distinguish different fundamental transport processes of the model [1].

[1] Ph. Stegmann, J. König, S. Weiss, submitted (2016)
[2] Ph. Stegmann, J. König, Phys. Rev. B **92**, 155413 (2015)
[3] Ph. Stegmann, J. König, Phys. Rev. B **94**, 125433 (2016)

TT 22.13 Tue 12:45 HSZ 103

Apparent pairing and subperiods in integer quantum Hall interferometers — •Giovanni Andrea Frigeri[1,3], Daniel Scherer[2], and Bernd Rosenow[3] — [1]Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany — [2]Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark — [3]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany

We analyze the magnetic field and gate voltage dependence of the conductance in an integer quantum Hall Fabry-Pérot interferometer, taking into account the interactions between an interfering edge mode, a non-interfering edge mode and the bulk. For weak bulk-edge coupling and sufficiently strong inter-edge interaction, we observe that the interferometer operates in the Aharonov-Bohm regime with a flux periodicity halved respect to the usual expectation. Even in the regime of strong bulk-edge coupling, this behavior can be observed as a subperiodicity of the interference signal in the Coulomb dominated regime. We do not find evidence for a connection between a reduced flux period and electron pairing, though. Our results can reproduce recent experimental findings.

TT 22.14 Tue 13:00 HSZ 103

Interplay of Hamiltonian control and and decoherence: a caveat, some hope and a new simulation strategy — •Jürgen Stockburger — Institute for Complex Quantum Systems, Ulm University

Hamiltonian control and decoherence are intricately intertwined in low-temperature quantum systems. For controls which act on timescales shorter than the thermal time $\hbar\beta$, Markovianity can no longer be assumed (RWA breakdown) [1]. When open-system dynamics is mapped on a stochastic propagation, this case can be treated exactly, and standard optimal control techniques can be used to explore synergy effects between control and reservoir interaction. Quantum states can thus be purified [2] and systems entangled [3] by the combined effect of local control and dissipation.

This stochastic mapping can now be combined with non-perturbative projection techniques, requiring only moderate computational resources [4].

[1] Alicki, R., Lidar, D. A. and Zanardi, P., Phys. Rev. A **73**, 052311 (2006)
[2] Schmidt, R. *et al.*, Phys. Rev. Lett. **107**, 130404 (2011)
[3] Schmidt, R., Stockburger, J. T. and Ankerhold, J., Phys. Rev. A **88**, 052321 (2013)
[4] Stockburger, J. T., EPL (Europhysics Letters) **115**, 40010 (2016)

TT 23: Transport: Topological Semimetals 1 (jointly with DS, MA, HL, O)

Time: Tuesday 9:30–11:45 Location: HSZ 201

TT 23.1 Tue 9:30 HSZ 201

Electron-hole pairing of Fermi arc surface states in a Weyl semimetal bilayer — •Paolo Michetti and Carsten Timm — Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

The topological nature of Weyl semimetals (WSMs) is corroborated by the presence of chiral surface states at the boundaries, connecting the bulk Fermi surface by Fermi arcs (FAs). We develop an analysis of the electron-hole pairing instability between the surface states of a bilayer structure realized by introducing a thin insulating spacer into a bulk WSM. We employ a minimal WSM model for the description of the surface states and a self-consistent mean-field treatment of the pairing interaction. We find that the system is unstable towards the formation of coherent electron-hole pairs, which leads to partial gapping of the FA dispersion curve and possibly to a superfluid dipolar exciton condensate, where dissipationless counter-propagating currents can be induced in the two layers. A signature of such condensate is the modifications of the peculiar quantum oscillations from surface FAs. We characterize the dependence of the single-particle energy gap and the critical temperature on the model parameters, where we emphasize in particular the linear scaling of these quantities with the separation between the Weyl points. A detrimental role is played by the curvature of the FA, although the phenomenon persists for moderately low curvature.

TT 23.2 Tue 9:45 HSZ 201

Universality and stability of the edge states of chiral nodal topological semimetals; Luttinger model for $j = \frac{3}{2}$ electrons as a 3D topological semimetal — •Maxim Kharitonov, Julian-Benedikt Mayer, and Ewelina Hankiewicz — Institute for Theoretical Physics and Astrophysics, Wuerzburg University

We theoretically demonstrate that the chiral structure of the nodes of nodal semimetals is responsible for the existence and universal local properties of the edge states in the vicinity of the nodes. We perform a general analysis of the edge states for an isolated node of a 2D semimetal, protected by *chiral symmetry* and characterized by the topological winding number N. We derive the asymptotic chiral-symmetric boundary conditions and find that there are $N+1$ universal classes of them. The class determines the numbers of flat-band edge states on either side off the node in the 1D edge spectrum and the winding number N gives the *total* number of edge states. We then show that the edge states of chiral nodal semimetals are *robust*: they persist in a finite-size *stability region* of parameters of chiral-asymmetric terms. This significantly extends the notion of 2D and 3D topological nodal semimetals. We demonstrate that the Luttinger model with a quadratic node for $j = \frac{3}{2}$ electrons is a 3D topological semimetal in this new sense and predict that α-Sn, HgTe, and possibly $Pr_2Ir_2O_7$, as well as many other semimetals described by it are topological and exhibit surface states.

TT 23.3 Tue 10:00 HSZ 201

Interband optical conductivity of the Dirac semimetal Cd_3As_2 — •D. Neubauer[1], J. P. Carbotte[2], A. A. Nateprov[3], A. Löhle[1], M. Dressel[1], and A. V. Pronin[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Department of Physics

and Astronomy, McMaster University, Canada — [3]Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau, Moldova

We measured the optical reflectivity of [001]-oriented n-doped Cd_3As_2 in a broad frequency range (50 – 22 000 cm^{-1}) for temperatures from 10 to 300 K. The optical conductivity, $\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)$, is isotropic within the (001) plane; its real part follows a power law, $\sigma_1(\omega) \propto \omega^{1.65}$, in a large interval from 2000 to 8000 cm^{-1}. This behavior is caused by interband transitions between two bands, which are effectively described by a sublinear dispersion relation, $E(k) \propto |k|^{0.6}$. The momentum-averaged Fermi velocity of the carriers in these bands is energy dependent and ranges from 1.2×10^5 to 3×10^5 m/s, depending on the distance from the Dirac points. These values are in agreement with the published data on Cd_3As_2. We detect a gaplike feature in $\sigma_1(\omega)$ and associate it with the Fermi level positioned around 100 meV above the Dirac points. Finally, we compare our results with recent magneto-optical infrared data.

TT 23.4 Tue 10:15 HSZ 201

Angular-dependent magnetoresistance of 3D Dirac materials — •Henry Legg and Achim Rosch — Institute for Theoretical Physics University of Cologne Zülpicher Straße 77 D-50937 Köln Deutschland

The realisation of 3D Dirac and Weyl semi-metals has created a new playground for transport phenomena, such as the possibility to produce the chiral anomaly in a condensed matter setting. Many materials that realise a 3D Dirac dispersion are protected by crystal symmetry and therefore have multiple Dirac cones within their Brillouin zone; examples include Cd_2As_2, Na_3Bi, and $Pb_{1-x}Sn_xSe$.

In this work we show that the application of a parallel magnetic and electric field in a direction perpendicular to that connecting a pair of Dirac cones can lead to a large positive magnetoresistance. The magnetic field leaves only an effective one-dimensional dispersion parallel to the field, due to the formation of Landau levels perpendicular to the magnetic field. The result is a large inter-nodal scattering matrix between the two Dirac cones since the Dirac nodes are close in the dimensionally reduced system. Our results are compared to recent experiments on $Pb_{1-x}Sn_xSe$.

15 min. break.

TT 23.5 Tue 10:45 HSZ 201

Quantum oscillation and Dirac fermion in $BaZnBi_2$ system — •Kan Zhao and Philipp Gegenwart — Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany

Dirac semimetals represent new quantum states of matter and have stimulated intensive studies. $AMnBi_2$(A = alkali earth/rare earth metal) is one of the established Dirac semimetals, with both antiferromagnetic order in $MnBi_4$ layer and Dirac fermion in Bi square net layer.

To investigate how the magnetism interacts with Dirac fermions, we synthesized single crystals of $SrZnBi_2$ and $BaZnBi_2$. Being isostructural to $SrMnBi_2$, $SrZnBi_2$ shows no quantum oscillation in resistivity and magnetic susceptibility up to 14 T. However, $BaZnBi_2$ shows clear multiple quantum oscillations down to 4 T in magnetic susceptibility. According to the temperature dependence of the oscillation amplitude after fast Fourier transformation (FFT), the effective electron mass is about 0.1me, comparable with that of $BaMnBi_2$. In the resistivity measurement up to 14 T at 2 K clear SdH oscillations with main oscillation frequency 168T are observed. The frequency follows a $1/|\cos(\theta)|$ dependence (θ is the angle between magnetic field and c axis), indicating a quasi 2D Fermi surface. Band-structure calculations by I. Mazin, indicate that $BaZnBi_2$ exhibits a unique structure feature and electronic structure, with a quasi Dirac band near the Fermi level. ARPES and high-field SdH measurements, to further characterize the Dirac fermions, are in progress.

TT 23.6 Tue 11:00 HSZ 201

Observation of Topological Surface States and Strong Electron/hole Imbalance in an Extreme Magnetoresistance Semimetal — •Niels Bernhard Michael Schröter[1], Juan Jiang[1,2,3,4], Shu-Chun Wu[5], Nitesh Kumar[5], Chandra Shekhar[5], Han Peng[1], Xiang Xu[6], Cheng Chen[1], Haifung Yang[7], Chan Hwang[4], Sung-Kwan Mo[3], Zhongkai Liu[2], Lexiang Yang[6], Claudia Felser[5], Binghai Yan[5], and Yulin Chen[1,2,6] — [1]University of Oxford, Oxford, UK — [2]ShanghaiTech University, Shanghai, P. R. China — [3]Advanced Light Source, Berkeley, USA — [4]Pohang Accelerator Laboratory, POSTECH, Pohang, Korea — [5]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [6]Tsinghua University, Beijing, P. R. China — [7]Chinese Academy of Sciences, Shanghai, P. R. China

The discovery of an extreme magnetoresistance (XMR) in the nonmagnetic rare-earth monopnictides LaX (X = P, As, Sb, Bi), a recently proposed new topological semimetal family, has inspired intensive research on the correlation between the XMR and their electronic structures. In this work, using ARPES to investigate the three dimensional band structure of a lanthanum monopnictide, we unraveled its topologically non-trivial nature with the observation of multiple topological surface Dirac fermions, as supported by our ab-initio calculations. Furthermore, we observed substantial imbalance between the volumes of electron and hole pockets, which rules out the electron-hole compensation as the primary cause of the XMR, putting strong constraints on future theoretical investigations.

TT 23.7 Tue 11:15 HSZ 201

Topological metal with multiple Dirac cones and nodal line — •Ashis Kumar Nandy[1], Alex Aperis[1], M. Mofazzel Hosen[2], Klauss Dimitri[2], Pablo Maldonado[1], Dariusz Kaczorowski[3], Tomasz Durakiewicz[4], Madhab Neupane[2], and Peter M. Oppeneer[1] — [1]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden — [2]Department of Physics, University of Central Florida, Orlando, Florida, USA — [3]Institute of Low Temp. & Structure Research, PAS, Wroclaw, Poland — [4]Condens. Matter and Magnet Science Group, LANL, Los Alamos, USA

The extended class of topological materials includes topological (semi) metals that support non-trivial topological surface states in the form of one-dimensional Dirac lines or Fermi-arcs connecting two Weyl points. Here we study a ternary compound using a combination of systematic theoretical calculations and detailed angle-resolved photoemission spectroscopy (ARPES) measurements. In contrast to other topological materials, our first-principles calculations suggest that the band inversion is $d-p$ type instead of the mostly observed $s-p$ type band inversion. We identify multiple Dirac fermionic states at various binding energies. A Dirac cone is computed at the Γ point about 0.5 eV above the chemical potential. Most importantly, at around 1 eV below the Fermi level our calculations reveal a surface nodal line-like feature passing through the time-reversal invariant point M. Our systematic study suggests a new family of materials for exploring the coexistence and competition of multiple fundamental fermionic quantum states.

TT 23.8 Tue 11:30 HSZ 201

PT **Anomalous Transport in a Nodal Line Dirac Semimetal** — •Wenbin Rui, Yuxin Zhao, and Andreas P. Schnyder — Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

Recently *PT* invariant topological nodal line Dirac semimetals have attracted increasing attentions in quantum matter. Here we study the anomalous transport of the *PT* symmetric Dirac semimetals of (3+1) dimensions as responses to electromagnetic fields, for which the universal currents are originated from the parity anomaly in (2+1)-dimensional quantum field theory. Considering that the total sum of anomalous currents from soft modes spreading along the nodal loop vanishes, we design a feasible experiment to detect the effect, which is able to separate anomalous currents from distinct regions of the nodal loop.

TT 24: Low-Dimensional Systems: 1D - Theory

Time: Tuesday 9:30–13:00 Location: HSZ 204

TT 24.1 Tue 9:30 HSZ 204

From Luttinger liquids to Luttinger droplets using higher-order bosonization identities — Sebastian Huber[1] and •Marcus Kollar[2] — [1]Theoretical Solid State Physics, Ludwig-Maximilians-University, Munich, Germany — [2]Theoretical Physics III, University of Augsburg, Germany

The exactly solvable Tomonaga-Luttinger model describes two flavors of interacting electrons with linear dispersion in one dimension, but some of its properties are characteristic for a wider class of one-dimensional systems according to the Luttinger liquid paradigm [1]. The exact solution for linear dispersion is based on bosonization, which represents fermionic particle-hole excitations in terms of canonical bosons and maps the Tomonaga-Luttinger Hamiltonian onto a free bosonic theory. We use the framework of constructive finite-size bosonization [2] to derive explicit bosonic representations of general bilinear fermion operators including arbitrary dispersion terms. As an application, Luttinger 'droplets' with position-dependent parameters are investigated.

[1] F. D. M. Haldane, J. Phys. C: Solid State Phys. **14**, 2585 (1981).
[2] J. von Delft and H. Schoeller, Ann. Phys. **7**, 225 (1998).

TT 24.2 Tue 9:45 HSZ 204

Interplay of Site and Bond Electron-Phonon Coupling in One Dimension — •Martin Hohenadler — University of Würzburg, Germany

The interplay of bond and charge correlations is studied in a one-dimensional model with both Holstein and Su-Schrieffer-Heeger (SSH) couplings to quantum phonons. The problem is solved exactly by quantum Monte Carlo simulations. If one of the couplings dominates, the ground state is a Peierls insulator with long-range bond or charge order. At weak coupling, the results suggest a spin-gapped and repulsive metallic phase arising from the competing order parameters and lattice fluctuations. Such a phase is absent from the pure SSH model even for quantum phonons. At strong coupling, evidence for a continuous transition between the two Peierls states is presented.

TT 24.3 Tue 10:00 HSZ 204

Effective narrow ladder model for metallic atomic nanowires on semiconducting substrates — •Anas Abdelwahab[1], Eric Jeckelmann[1], and Martin Hohenadler[2] — [1]Leibniz Universität Hannover, Germany — [2]Universität Würzburg, Germany

We perform a systematic construction of an effective quasi-one-dimensional ladder model starting from a 3D wire-substrate model. This construction depends on an exact mapping of the full 3D wire-substrate model onto a 2D ladder model, followed by a truncation to a ladder with a limited number of legs to approximate the full wire-substrate model. For insulating (but not for metallic) substrates, ladders with at least three legs are found to give a good qualitative approximation. We discuss the influence of wire-substrate hybridization on a wire described by the 1D Hubbard model. We observe several phases such as Mott insulator, Luttinger liquid, band insulator, and Fermi liquid. The effective ladder model is suggested to describe correlation effects in systems of metallic atomic nanowires deposited on semiconducting substrates.

Support from the DFG through the Research Units FOR 1700 and FOR 1807 as well as SFB 1170 is gratefully acknowledged.

TT 24.4 Tue 10:15 HSZ 204

Filling-dependent doublon dynamics in the one-dimensional Hubbard model — •Roman Rausch and Michael Potthoff — I. Institute for Theoretical Physics, University of Hamburg

The fate of a local two-hole doublon excitation in the one-dimensional Fermi-Hubbard model is systematically studied in the entire filling range using the density-matrix renormalization group (DMRG) and the Bethe ansatz. For strong Hubbard interaction U, two holes at the same site form a compound object whose decay is impeded by the lack of phase space. Still, a partial decay is possible on an extremely short time scale where phase-space arguments do not yet apply. We argue that the initial decay and the resulting intermediate state are relevant for experiments performed with ultracold atoms loaded into an optical lattice as well as for CVV Auger-electron spectroscopy. The discussion comprises the mixed ballistic-diffusive real-time propagation of the doublon through the lattice, its partial decay on the short time scale as a function of filling and interaction strength, as well as the analysis of the decay products, which are metastable on the intermediate time scale. The ambivalent role of singly occupied sites is key to understanding the doublon physics: For high fillings, ground-state configurations with single occupancies are recognized to strongly relax the kinematic constraints and to open up decay channels. For fillings close to half filling, however, their presence actually blocks the doublon decay. Finally, we demonstrate that the decay products as well as the doublon propagation should rather be understood in terms of Bethe ansatz eigenstates (spinons and holons).

TT 24.5 Tue 10:30 HSZ 204

Thermal Intra-Band Magnon Scattering in the Haldane Spin-One Chain — •Jonas Becker[1], Thomas Köhler[2], Alexander C. Tiegel[2], Salvatore R. Manmana[2], Andreas Honecker[3], and Stefan Wessel[1] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, 52056 Aachen, Germany — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [3]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, Université de Cergy-Pontoise, F-95302 Cergy-Pontoise Cedex, France

We present results from a thorough evaluation of the dynamical spin structure factor of the Haldane chain at finite temperatures, based on a combination of exact numerical diagonalization, finite-temperature density-matrix renormalization group calculations and quantum Monte Carlo simulations. Simulations performed on finite open chains exhibit a sub-gap band in the thermal spin spectral function, indicative of the localized edge-modes in the Haldane chain's ground state. Furthermore, we observe the thermal activation of a distinct low-energy contribution to the spin spectral function with an enhanced spectral weight at low momenta that results from intra-band magnon scattering due to the thermal population of the single-magnon mode. These findings are discussed with respect to previous results on the spin spectral function and possible future studies on Haldane spin chain compounds based on inelastic neutron scattering experiments.

TT 24.6 Tue 10:45 HSZ 204

Photoexcitations in a 1D manganite model: From quasiclassical light absorption to quasiparticle relaxations — •Thomas Köhler[1], Sangeeta Rajpurohit[2], Ole Schumann[1], Fabian Biebl[1], Mohsen Sotoudeh[2], Stephan Kramer[3,1], Peter Blöchl[2,1], Stefan Kehrein[1], and Salvatore Manmana[1] — [1]Inst. f. Theo. Phys., U. Göttingen — [2]Inst. f. Theo. Phys., TU Clausthal — [3]Fraunhofer ITWM Kaiserslautern

We investigate the dynamics of 1D correlated systems after photoexcitation by combining ab-initio methods, time-dependent matrix product states (MPS), linearized quantum Boltzmann equations (LBE), and molecular dynamics (MD) simulations. This leads to a description spanning a wide range of time scales from femto- up to nanoseconds. We consider manganite systems in the material class $Pr_{1-x}Ca_xMnO_3$ for which we derive 1D ab-initio model Hamiltonians. At half doping, we obtain a magnetic microstructure of alternating dimers from which we derive a 1D Hubbard-type model. The dynamics is analyzed concerning the formation and lifetime of such quasiparticles via a LBE. We find that the magnetic microstructure strongly enhances the lifetime of the excitations. In this way, our work constitutes a first step to building a unifying theoretical framework for the description of photoexcitations in strongly correlated materials over a wide range of time scales, capable of making predictions for ongoing experiments investigating pump-probe situations and unconventional photovoltaics.

Financial support by DFG CRC1073 (projects B03 and C03) is gratefully acknowledged.

15 min. break.

TT 24.7 Tue 11:15 HSZ 204

Scattering of an electronic wave packet by a one-dimensional electron-phonon-coupled structure — •Christoph Brockt and Eric Jeckelmann — Leibniz Universität Hannover, Germany

We investigate the scattering of an electronic wave packet by phonons within the one-dimensional Holstein model. The electron-phonon cou-

pling is confined in a small structure between two tight-binding leads. We observe permanent energy transfer from the electron to the phonon system, transient self-trapping of the electron in the electron-phonon coupled structure and transmission resonances, that depend on the adiabaticity ratio.

A recently developed TEBD algorithm [1], that uses optimal modes [2] for the bosonic degrees of freedom, was used for this study. Analytical results are provided for a single-site electron-phonon coupled structure and for limiting cases.

Support from the DFG through the Research Unit FOR 1807 is gratefully acknowledged.

[1] C. Brockt et al., PRB **92**, 241106 (2015)
[2] C. Zhang, E. Jeckelmann, and S.R. White, PRL **80**, 2661 (1998)

TT 24.8 Tue 11:30 HSZ 204

DMRG method for the conductance of one-dimensional correlated systems — •Jan Bischoff — Leibniz Universität Hannover

We present an accurate and efficient procedure for computing the zero-temperature linear conductance of correlated one-dimensional systems using the density-matrix renormalization group (DMRG). Building on [1], we express the conductance within the linear response theory as the limits of dynamical correlation functions for finite systems. These correlation functions can be calculated with the dynamical DMRG algorithm. We have first studied non-interacting models to determine an appropriate scaling of frequency, system size, and spectral broadening by comparison with exact results. The method is demonstrated for interacting systems using the one-dimensional spinless fermion model. Our results for this lattice model agree with the field-theoretical predictions for the renormalization of the conductance in a pure Luttinger liquid as well as for the effects of an impurity in a Luttinger liquid [2]. We have found that this new approach is more efficient than a simulation of the nonequilibrium transport [3] in the linear response regime. We have also tested our approach on the Hubbard model and we plan to extend it to the problem of an interacting quantum wire connected to two broad and weakly-interacting leads.

[1] D. Bohr, P. Schmitteckert, and P.W. Wölfle, Europhys. Lett., 73, 246 (2006)
[2] C.L. Kane and M.P.A. Fisher, PRB 46, 15233 (1992)
[3] M. Einhellinger, A. Cojuhovschi, and E. Jeckelmann, Phys. Rev. B 85, 235141 (2012)

TT 24.9 Tue 11:45 HSZ 204

Thermal transport in Kitaev–Heisenberg ladders — •Alexandros Metavitsiadis and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Braunschweig, Germany

We study the finite temperature thermal transport properties of a Kitaev–Heisenberg two leg ladder, as a minimum quasi one–dimensional representative of the corresponding two–dimensional model on a Honeycomb lattice. In the absence of Heisenberg interactions, we find that the pure Kitaev ladder is an ideal heat insulator at all temperatures. This is a direct consequence of the fractionalization of spin degrees of freedom which acts as a thermally activated disorder leading to localization. On the other hand, Heisenberg interactions restore DC conductivity, driving the system into a conducting state where transport is mediated by triplon excitations. We primarily rely on numerical techniques, namely exact diagonalization and the quantum typicality.

TT 24.10 Tue 12:00 HSZ 204

Nonequilibrium energy dynamics in the spin-$\frac{1}{2}$ XXZ chain — •Younes Javanmard[1], Soumya Bera[1], and Jens H. Bardarson[1,2] — [1]Max Planck Institute for Physics of Complex Systems, Dresden, Germany — [2]Department of Theoretical Physics, KTH Royal Institute of Technology, Stockholm, Sweden

We study the real-time dynamics of spin-$\frac{1}{2}$ XXZ chains out of thermal equilibrium using time evolving block decimation algorithms. We consider both integrable and non-integrable systems at and away from half-filling, focussing on the analysis of the time-dependent behavior of the local energy density profile and current.

TT 24.11 Tue 12:15 HSZ 204

Microscopic Analysis of 1D Lattice Models for Synthetic Helical Liquids — •Lorenzo Pastori and Jan Carl Budich — Department of Physics, University of Gothenburg, SE 412 96 Gothenburg, Sweden

Helical liquids exhibiting spin-momentum locking are known to appear at the edges of 2D time-reversal invariant topological insulators. Here we investigate various Fermi-Hubbard models for 1D lattice systems where synthetic helical liquids can be realised. In such models the low-energy physics around the Fermi points can be described in terms of emergent helical Luttinger liquid behaviour. Using density matrix renormalisation group techniques, we quantitatively analyse the presence of spin-momentum locking, i.e. the key hallmark of helical liquids, by studying ground state spin-spin correlation functions.

TT 24.12 Tue 12:30 HSZ 204

Role of Cu 4*d* and O 3*p* orbitals in the many-body wavefunction of corner-sharing cuprates — •Nikolay A. Bogdanov[1], Giovanni Li Manni[1], Sandeep Sharma[1], Olle Gunnarsson[1], and Ali Alavi[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University Chemical Laboratory, Cambridge, U.K.

Electronic and magnetic properties of one- and two-dimensional cuprates have been investigated for several decades but are still not fully understood. We study the electronic structure of the undoped Sr_2CuO_3 and La_2CuO_4 corner-sharing cuprates with state-of-the-art wavefunction-based *ab initio* calculations. We find that in order to obtain reasonable agreement with the experimentally observed large magnetic exchange couplings for these compounds, it is necessary to go beyond multiband models containing only Cu 3*d* and O 2*p* bands. To capture the orbital breathing effects it is necessary to extend the model space with diffuse Cu 4*d* and O 3*p* orbitals. For a Cu-O-Cu unit this leads to a problem of 24 electrons in 26 orbitals that can't be solved with conventional methods. In our study we employ full configuration interaction quantum Monte Carlo (FCIQMC) and density matrix renormalization group (DMRG) techniques to tackle this problem.

TT 24.13 Tue 12:45 HSZ 204

Topological mirror insulators in one dimension — •Alexander Lau[1], Jeroen van den Brink[1,2], and Carmine Ortix[1,3] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [2]Institute for Theoretical Physics, TU Dresden, Germany — [3]Institute for Theoretical Physics, Utrecht University, Netherlands

In the context of novel topological states of matter protected by crystalline symmetries, we show that the presence of mirror symmetry leads to a new class of time-reversal invariant topological insulators in one dimension. These *topological mirror insulators* are characterized by a nontrivial $\mathbb{Z}_2$ topological invariant defined in terms of the partial polarization, which we show to be quantized in the presence of a 1D mirror point. Their hallmark is an odd number of electronic integer end charges at the mirror-symmetric boundaries of the system.

We check our findings against spin-orbit coupled Aubry-André-Harper models which realize this novel topological state of matter. The presented models could be realized, for instance, in cold-atomic Fermi gases loaded in periodic optical lattices.

TT 25: Correlated Electrons: Frustrated Magnets - Strong Spin-Orbit Coupling 1

Time: Tuesday 9:30–13:00 Location: HSZ 304

TT 25.1 Tue 9:30 HSZ 304

Quantum spin liquid ground state in $Ba_3InIr_2O_9$: A combined NMR and μSR study — •Mayukh Majumder[1], Tusharkanti Dey[1], Jean-Christophe Orain[2], Norbert Buettgen[3], Alexander Tsirlin[1], and Philipp Gegenwart[1] — [1]EP-VI, EKM, University of Augsburg, Germany — [2]Paul Scherrer Institute, Switzerland — [3]EP-V, EKM, University of Augsburg, Germany

5*d* Iridium based systems have drawn a lot of attention because of the presence of similar energy scales of crystal field splitting, spin-orbit coupling and on-site Coulomb interaction which give rise to unconventional ground states. In the present compound $Ba_3InIr_2O_9$ (Ir has an average of +4.5 oxidation state), Ir-dimers aligned along crystallographic c-axis form a triangular lattice which promotes frustration. The magnetization and specific heat show no evidence of long-range magnetic ordering down to 400 mK. We have employed ^{115}In (I=9/2) NMR and μSR to study the microscopic nature of the ground state. ^{115}In Knight shift and line width exhibit a temperature independent behavior below 1.4 K down to 25 mK which indicates no static correlations are developing down to such a low temperature whereas the nuclear spin-lattice relaxation rate ($1/T_1$) shows a dynamical behavior in the same temperature range and follows a $T^{2.2}$ power law. Furthermore, we have carried out μSR experiments which also discarded the presence of any static long-range ordering and provide the evidence of dynamical fluctuations down to 25 mK. Altogether, local probes provide strong evidence for gapless quantum spin liquid ground state in $Ba_3InIr_2O_9$.

TT 25.2 Tue 9:45 HSZ 304

Spin liquid behavior in the triangular lattice iridate $Ba_3InIr_2O_9$ — •Tusharkanti Dey[1], Mayukh Majumder[1], Anatoliy Senyshyn[2], Panchanan Khuntia[3], Alexander Tsirlin[1], and Philipp Gegenwart[1] — [1]EP-VI, EKM, University of Augsburg, Germany — [2]Munich University of Technology, Germany — [3]Universite Paris-Sud, Orsay, France

Materials with the general formula $Ba_3MIr_2O_9$ (M is a trivalent ion) crystallize in a hexagonal structure containing face-sharing Ir_2O_9 bi-octahedra forming Ir-Ir dimers along the crystallographic c-axis. These dimers build a triangular lattice in the crystallographic ab-plane. In these materials, Ir has a single crystallographic site with an average charge state +4.5. Therefore the two Ir sites within the dimer share one electron among them. This fractional charge state combined with the frustrated geometry give rise to many interesting properties like magnetoelastic effect, spin gap behavior and magnetic ordering. We have recently synthesized polycrystalline sample of $Ba_3In^{3+}Ir^{4.5+}{}_2O_9$ and studied its structural, magnetic and thermodynamic properties in detail. Our magnetic susceptibility data show the absence of magnetic ordering down to 0.4 K which is very small compared to the Weiss temperature. The magnetic heat capacity shows a hump at 1.6 K and follows power law with temperature below 1 K. In this presentation, we will discuss these results suggesting a quantum spin liquid ground state for this material.

TT 25.3 Tue 10:00 HSZ 304

Magnetism of honeycomb ruthenate $Ag_3LiRu_2O_6$ without singlet dimers — •Tomohiro Takayama[1,2] and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]FMQ3, University of Stuttgart, Stuttgart, Germany — [3]Department of Physics, University of Tokyo, Tokyo, Japan

Honeycomb-based transition-metal oxides currently attract interests as novel quantum magnets. 5*d* honeycomb iridates were theoretically proposed to host quantum spin liquid state owing to bond-dependent magnetic coupling (Kitaev coupling)[1], and experimental verifications of such spin liquid state are intensively under way. On the other hand, honeycomb ruthenate Li_2RuO_3 is known to form spin-singlet dimers and the ground state is non-magnetic insulator [2].

By using ion-exchange reaction, we have synthesized silver-intercalated honeycomb ruthenate $Ag_3LiRu_2O_6$ [3]. Possibly due to the formation of strong O^{2-}-Ag^{+}-O^{2-} between the honeycomb layers, the singlet-dimer formation is suppressed in $Ag_3LiRu_2O_6$, and Ru^{4+} magnetism survives down to low temperatures. Despite Curie-Weiss like behavior observed at high temperatures (θ_{CW} $\sim$ -40 K), we did not see any magnetic order down to 2 K in magnetization and heat capacity measurements. We discuss the possible magnetic ground state of this honeycomb ruthenate.

[1] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. 102, 017205 (2009)
[2] Y. Miura et al., J. Phys. Soc. Jpn., 76, 033705 (2007)
[3] S. Kimber et al., J. Mater. Chem. 20, 8021 (2010)

TT 25.4 Tue 10:15 HSZ 304

Long-range interactions in the effective low energy Hamiltonian of Sr_2IrO_4: a core level resonant inelastic x-ray scattering — •Stefano Agrestini[1], Chang-Yang Kuo[1], Marco Moretti Sala[2], Zhiwei Hu[1], Deepa Kasinathan[1], Pieter Glatzel[2], Tomohiro Takayama[3,4], Hidenori Takagi[3,4,5], Liu Hao Tjeng[1], and Maurits W. Haverkort[1,6] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]ESRF, Grenoble, France — [3]Department of Physics and Department of Advanced Materials, University of Tokyo, Japan — [4]Max Planck Institute for Solid State Research, Stuttgart, Germany — [5]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany — [6]Institute for theoretical physics, Heidelberg University, Germany

The iridates have received tremendous attention due to the high expectations of finding new exotic phenomena and the long-sought materialization of the Kitaev model. Experimentally, however, most compounds order magnetically. Here we address the puzzle of the ground state in iridates by measuring core-to-core resonant inelastic x-ray spectroscopy on Sr_2IrO_4. From the spectra analysis we found that Sr_2IrO_4 is highly covalent with the effective t_{2g} orbitals very extended spatially. They are not the standard orbitals with nearest-neighbor-only magnetic interactions that most people have in mind. We thus explain why compass models are not realized in most studied iridates and we show a pathway how one can achieve the Kitaev model using other crystal structures or transition metal ions.

TT 25.5 Tue 10:30 HSZ 304

Differences in motion of a single hole and a single electron in the quasi-2D iridates — •Ekaterina Paerschke[1], Krzysztof Wohlfeld[2], Kateryna Foyevtsova[3], and Jeroen van den Brink[1] — [1]IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland — [3]University of British Columbia, 6224 Agricultural Road, Vancouver, BC V6T 1Z1 Canada

We study the motion of a single charge (hole or electron) added to the (Mott) insulating and antiferromagnetically ordered ground state of the quasi-2D iridates, such as Ba_2IrO_4 or Sr_2IrO_4. Using the self-consistent Born approximation applied to the appropriate strong coupling model we show the intrinsic and qualitative differences between the hole and electron cases. On one hand, the added electron forms a spin polaron, which qualitatively resembles the well-known case of the quasi-2D cuprates doped with a single hole or electron. On the other hand, the case with the added hole is far more complex, due to the formation of the $5d^4$ configuration which may carry finite angular momentum J: here the well-known spin polaronic physics is modified due to the additional degrees of freedom and the possibility of the free hole motion between the different AF sublattices. These results have important consequences not only for the photoemission experiments of the undoped quasi-2D iridates but also suggest that the physics of the electron- and hole-doped iridates is fundamentally different.

TT 25.6 Tue 10:45 HSZ 304

Electronic structure of Sr_2IrO_4 probed with low temperature scanning tunneling microscopy — Zhixiang Sun, •Jose M. Guevara, Danny Baumann, Kaustuv Manna, Sabine Wurmehl, Bernd Büchner, and Christian Hess — IFW-Dresden, Helmholtzstrasse 20, 01069

Sr_2IrO_4 is the main example of a spin-orbit assisted Mott insulator. In the family of iridates, Sr_2IrO_4 has also been postulated as a candidate to emulate the physics of the parent compound of the high-temperature superconductors cuprates, where the doping effect in the insulator to metal transition is still not well understood.

In this work, we classify different predominant defects in Sr_2IrO_4, with low temperature STM/S. We probe the spatial structure symmetry of these defects. From the tunneling spectra, we identify the energy of the upper and lower $J_{eff} = 1/2$ Hubbard bands, the Mott gap, and the variation of the electronic structure due to defects. A charge transfer-like behavior for the defect caused ingap states is observed.

Our measurements provide detailed results about the defect effects to the electronic properties of Sr_2IrO_4, which can be important for further understanding of the doping effect in iridates and the insulator to metal transition in Mott insulators.

TT 25.7 Tue 11:00 HSZ 304

New pyrochlore iridate $In_2Ir_2O_7$ stabilised by high pressure — •Aleksandra Krajewska[1,2], Tomohiro Takayama[1,2], Robert Dinnebier[2], Alexander Yaresko[2], Kenji Ishii[3], and Hidenori Takagi[1,2] — [1]Institut für Funktionelle Materie und Quantentechnologien, University of Stuttgart, 70550 Stuttgart, Germany — [2]Max-Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [3]QST, Hyogo 679-5148, Japan

In 5*d* transition metal oxides Coulomb repulsion, crystal field splitting and spin-orbit coupling are comparable which leads to a variety of exotic electronic states. Pyrochlore iridates with chemical formula $A_2Ir_2O_7$ (A= Y, rare earth) consist of A and Ir corner-sharing tetrahedral networks and are predicted to exhibit Weyl semimetal or topological insulator states. Their properties depend on the ionic radius of A^{3+}, where the system is driven from metallic to insulating regime with decreasing A^{3+} size. Those effects are likely related to diverging degree of local lattice distortion. In our work in order to explore small A^{3+} limit we synthesised new pyrochlore $In_2Ir_2O_7$ using high pressure. Structural analysis shows its octahedra are the most distorted among $A_2Ir_2O_7$ family which is in agreement with its insulating behaviour. It shows magnetic order at $T_N = 55$ K with $\theta_{CW} \sim$ -400 K, which suggests strong frustration and is in large contrast with $Y_2Ir_2O_7$ (T_N = 155 K, $\theta_{CW} \sim$ -130 K). Our band calculation shows that despite large distortion $In_2Ir_2O_7$ is in proximity to pure $j_{eff} = 1/2$, unlike $Y_2Ir_2O_7$, which shows strong hybridisation of $j_{eff} = 1/2$ and $j_{eff} = 3/2$. We will discuss the possible origin of almost pure $j_{eff} = 1/2$ state in $In_2Ir_2O_7$.

15 min. break.

TT 25.8 Tue 11:30 HSZ 304

Magnetic ground state of the pyrochlore iridate $Nd_2Ir_2O_7$ — •Hanjie Guo[1], Clemens Ritter[2], Kazuyuki Matsuhira[3], Isao Watanabe[4], Liu Hao Tjeng[1], and Alexander Komarek[1] — [1]MPI CPfS, Dresden, Germany — [2]ILL, Grenoble, France — [3]Kyushu Institute of Technology, KitaKyushu, Japan — [4]RIKEN, Wako, Japan

Pyrochlore iridates are of interest due to the interplay between the relatively large spin-orbit coupling and electron-electron correlations which may induce novel phases such as Weyl semimetals. One important task for understanding the properties of these compounds is the determination of the magnetic structure which is challenging due to the small size of Ir^{4+} moments and maybe also due to the neutron absorption from Ir atoms. Our μSR studies on $Nd_2Ir_2O_7$ clearly show two transitions below about 30 and 9 K related to the Ir and Nd sublattices, respectively. The full magnetic structure including the Ir sublattice has been determined by means of powder neutron diffraction at the high flux D20 diffractometer at the ILL. Our magnetic structure refinement unravels a so-called all-in/all-out magnetic structure for both the Nd and the Ir sublattices. The ordered magnetic moments at 1.8 K amount to 0.34(1) μ_B/Ir^{4+} and 1.27(1) μ_B/Nd^{3+}.

[1] H. Guo, C. Ritter and A. C. Komarek, Phys. Rev. B **94**, 161102(R) (2016).

TT 25.9 Tue 11:45 HSZ 304

Synthesis and magnetic properties of double perovskites with Ir(IV)-states — •Michael Vogl[1], Tusharkanti Dey[1,2], Laura Teresa Corredor Bohorquez[1], Saicharan Aswartham[1], Anja Wolter-Giraud[1], Sabine Wurmehl[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research , Dresden, Germany — [2]EP-VI, Electronic Correlations and Magnetism, University of Augsburg, Germany

With strong spin-orbit coupling 5d-based iridates exhibit many interesting phenomena and ground states. Here, we synthesized and investigated two series of 5d-based double perovskites $La_2Co_{1-x}Zn_xIrO_6$ and $La_2Cu_{1-x}Zn_xIrO_6$. Polycrystalline samples of the substitution series were synthesized by conventional solid state reaction and characterized by structural, magnetic and specific heat measurements. In both parent compounds (x=0) complex magnetic interactions between the strongly spin-orbit coupled 5d-ion Ir^{4+} and a magnetic 3d-transition metal ion (Co/Cu) are present. Dilution with non-magnetic Zn^{2+} is used to further study this interaction.

The evolution of the magnetic properties throughout both series is discussed. A strong shift of the transition temperatures to lower temperatures can be observed with increasing Zn-content. The magnetic phase diagram for both the series is mapped out.

TT 25.10 Tue 12:00 HSZ 304

Correlating paramagnetic spin centers in the 'nonmagnetic' $5d^4$ compound Ba_2YIrO_6 — •Stephan Fuchs[1], Vladislav Kataev[1], Franziska Hammerath[1], Gizem Aslan Cansever[1], Tushar Dey[1], and Bernd Büchner[1,2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden,D-01171 — [2]Institut für Festkörperphysik, Technische Universität Dresden,D-01062

We will present the electron spin resonance results of the double perovskite Ba_2YIrO_6. This material provides a playground to examine the magnetic interactions in a 5d transition metal oxide with strong spin-orbit coupling. Theory predicts that due to the strong spin-orbit coupling this $5d^4$ iridate should be in a nonmagnetic state. However, static magnetic and NMR measurements evidence the occurrence of paramagnetic spin centers that are correlated at low temperatures. To obtain deeper insight into the magnetic properties of Ba_2YIrO_6 ESR measurements of a polycrystalline sample were carried out for several temperatures and frequencies. This enables to quantify several different paramagnetic spin centers. Two of them correspond to S=1/2 with the g-factor g=1.99 and g=1.90, and the third one to S=3/2 with g=1.49. An overview of the possible origins for the different spin centers and their relevance to the unexpected magnetism of this compound will be given in this talk.

TT 25.11 Tue 12:15 HSZ 304

The iridium double perovskites with Ir^{5+} revised: a combined structural and specific heat study — •Mihai I. Sturza[1], Laura T. Corredor[1], Gizem Aslan Cansever[1], Kaustuv Manna[1], Sebastian Gass[1], Tushar Dey[1], Christian Blum[1], Andrey Maljuk[1], Olga Kataeva[2], Sabine Wurmehl[1], Anja Wolter[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research IFW, Institute for Solid State Research, 01069 Dresden, Germany — [2]A.E. Arbuzov Institute of Organic and Physical Chemistry, Russian Academy of Sciences, Kazan, Russia

Recently, the iridate double perovskite Sr_2YIrO_6 has attracted considerable attention due to the report of unexpected magnetism in this Ir^{5+} material, in which according to the Jeff model, a non-magnetic ground state is expected. We present a structural, magnetic and thermodynamic characterization of Sr_2YIrO_6 and Ba_2YIrO_6 single crystals, with emphasis on the temperature and magnetic field dependence of the specific heat. In agreement with the expected non-magnetic ground state of Ir^{5+} ($5d^4$) in these iridates, no magnetic transition is observed down to 430 mK. Moreover, our results suggest that the low temperature anomaly observed in the specific heat is not related to the onset of long-range magnetic order. Instead, it is identified as a Schottky anomaly caused by paramagnetic impurities present in the sample, of the order of 0.5(2) %. These impurities lead to non-negligible spin correlations, which nonetheless, are not associated with long-range magnetic ordering.

TT 25.12 Tue 12:30 HSZ 304

Strain induced changes of electronic properties of B–site ordered Sr_2CoIrO_6 thin films — •Sebastian Esser[1], Chun-Fu Chang[2], Vladimir Roddatis[3], Vasily Moshnyaga[4], Liu Hao Tjeng[2], and Philipp Gegenwart[1] — [1]Experimentalphysik VI, Universität Augsburg, 86159 Augsburg, Germany — [2]Max Planck Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [3]Institut für Materialphysik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [4]1. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Tight-binding calculations for perovskite $SrIrO_3$ indicate a line node near the Fermi energy. Introducing a staggered potential between the iridate layers should gap out the nodal line, leaving a pair of three-dimensional nodal points [1] and providing a strong motivation to synthesize B–site ordered double perovskite iridate materials.

By using a metal-organic aerosol deposition technique we have grown

Sr_2CoIrO_6 thin films on various (pseudo) cubic (001)-oriented substrates to investigate the strain induced changes of the electronic properties. The fully epitaxial strained state of the thin films was verified by x-ray diffraction patterns in combination with reciprocal space mapping and TEM images. HAXPES measurements at SPring-8 indicating a strain induced change of the valence band in the near of the Fermi edge. These changes are also affecting the electrical transport properties, which were investigated down to lowest temperatures.

This work is supported by the German Science foundation through SPP 1666.

[1] J.-M. Carter *et al.*, Phys. Rev. B **85** (2012) 115105.

TT 25.13 Tue 12:45 HSZ 304

Frustrated magnetism and Kitaev exchange on the fcc lattice of K_2IrCl_6 — •Nazir Khan and Alexander A. Tsirlin — EP VI, EKM, Augsburg University, 86159 Augsburg, Germany

Face-centered cubic lattice (fcc) is inherently frustrated, whereas Ir^{4+} ion brings the possibility of Kitaev anisotropy. Synchrotron x-ray study on the powder sample of K_2IrCl_6 shows that the compound retains its room temperature fcc structure (space group Fm-$3m$) and symmetrical Cl_6 octahedral environment down to the low temperature of 20 K followed by 3% volume collapse of the unit cell. Temperature and field dependence of magnetization show that the compound undergoes a paramagnetic to an antiferromagnetic phase transition at T_N=3.14 K. The Curie-Weiss fitting to the high temperature data yields an effective magnetic moment μ_{eff} =1.69 μ_B/Ir ion and Curie-Weiss temperature θ_{CW}=−41.0 K. The frustration parameter, $f = |\theta_{CW}|/T_N$, is found to be 13.0 which suggests presence of significant magnetic frustration. The temperature dependence of electrical resistivity shows that the compound is an insulator with a charge gap close to 0.7 eV.

TT 26: Two-Dimensional Materials III (joint session DS, HL, TT, organized by HL)

Time: Tuesday 9:30–13:15 Location: POT 51

TT 26.1 Tue 9:30 POT 51

Optical properties of organic/inorganic and all-inorganic lead halide perovskite nanoplatelets — •Jasmina A. Sichert[1,2], Yu Tong[1,2], Verena A. Hintermayr[1,2], Alexander F. Richter[1,2], Bernhard Bohn[1,2], Lakshminarayana Polavarapu[1,2], Carlos Cardenas-Daw[1,2], Alexander S. Urban[1,2], and Jochen Feldmann[1,2] — [1]Chair for Photonics and Optoelectronics, Department of Physics and Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität (LMU), Amalienstaße 54, 80799 Munich, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 Munich Germany

In recent years, organic/inorganic and all-inorganic lead halide perovskite have shown great potential for photovoltaics as well as for light-emitting applications. We have successfully synthesized two-dimensional methylammonium and cesium lead halide perovskite nanoplatelets of varying thickness down to one monolayer.[1,2] With decrease in crystal thickness we observed quantum-size effects and an increase in the exciton binding energy. In the extreme case of a perovskite sheet only a single unit cell thick, the screening of the exciton decreases significantly, resulting in a huge exciton binding energy of several hundred meV in the thin nanoplatelets. We conducted time-resolved photoluminescence spectroscopy to further investigate the effect of the crystal thickness on the optical properties of the nanoplatelets.

[1] Sichert et al., Nano Lett. 15, 6521-6527 (2015)
[2] Tong et al., Angew. Chem. 55, 13887-13892 (2016)

TT 26.2 Tue 9:45 POT 51

Band-gap and exciton binding-energy renormalizations due to excited carriers in monolayer TMDs — •Daniel Erben[1], Christopher Gies[1], Malte Rösner[1,2], Alexander Steinhoff[1], Matthias Florian[1], Michael Lorke[1], Tim Wehling[1,2], and Frank Jahnke[1] — [1]Insitute for Theoretical Physics, University of Bremen, Germany — [2]Bremen Center for Computational Materials Science, University of Bremen, Germany

Coulomb interaction between charge carriers in atomically thin layers of transition-metal dichalcogenides (TMDs) has been shown to be exceptionally large due to the weak screening in the thin layer itself. It causes strong renormalization effects which change the electronic properties and the optical response of the material.

We investigate excited-state optical properties of the typical monolayer TMDs MoS_2, $MoSe_2$, WS_2 and WSe_2 by solving the semiconductor Bloch equations on the full Brillouin zone using the SXCH-approximation for the Coulomb interaction. Excitonic resonances shift in absolute value and relative to each other with increasing carrier density. This effect is a result of a band-gap reduction due to many-particle renormalizations and a reduction of the binding energy due to screening of the Coulomb interaction and Pauli blocking, which we analyse and compare in detail for MoS_2, $MoSe_2$, WS_2 and WSe_2. Our calculations predict a transition from a direct to an indirect band-gap in molybdenum and tungsten disulfides in the presence of highly excited carriers. The selenides stay indirect for different excitations.

TT 26.3 Tue 10:00 POT 51

Phase separation and composition fluctuation effects on electronic and optical properties of $(BN)_{1-x}(C_2)_x$ 2D alloy — •Ivan Guilhon[1], Lara K Teles[1], Marcelo Marques[1], and Friedhelm Bechstedt[2] — [1]Grupo de Materiais Semicondutores e Nanotecnologia, Instituto Tecnológico de Aeronáutica, DCTA, 12228-900 São José dos Campos, Brazil — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, D-07743 Jena, Germany

$(BN)_{1-x}(C_2)_x$ alloys are promising materials for band gap engineering in two-dimensional electronics. Despite the importance of microstructural features, such as phase separation and composition fluctuation. The current theoretical studies of such monolayer alloys are often restricted to investigate "guessed" nonrandom structures.

Using DFT calculations combined with a statistical approach to account for disorder effects, we study the properties of these 2D alloys as a function of their average composition. A complete scenario of how thermodynamic conditions affect the distribution of atoms is provided. The solubility limits and critical temperature are studied by constructing a T-x phase diagram.

In this context, we calculate the energy gap as a function of the composition and optical absorbance spectra are predicted for different compositions. Our predictions are compared with the experimental findings. We reproduce the experimentally found absorption spectra with a two-peak pattern for intermediate carbon concentrations and identify them with phase-segregated instead of homogeneous alloys.

TT 26.4 Tue 10:15 POT 51

Electron-phonon interaction in transition metal dichalcogenides — •Nicki F. Hinsche[1], Arlette Sohanfo Ngankeu[2], Sanjoy Mahatha[2], Marco Bianchi[2], Charlotte Sanders[2], Philip Hofmann[2], and Kristian S. Thygesen[1] — [1]Center for Atomic-scale Materials Design, Technical University of Denmark, 2830 Kgs. Lyngby, Denmark — [2]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark

Atomically thin layers of Transition Metal Dichalcogenides (TMD) attract remarkable interest due to their extraordinary electronic and optical properties and are often quoted as semiconductor analogues of graphene. Possessing direct band gaps in the visible frequency range and exhibiting high electronic mobilities at room temperature, TMD's are emerging candidates for next generation electronic and optoelectronic applications [1]. By means of DFT electronic-structure and Boltzmann transport calculations [2], we discuss the impact of microscopic electron-phonon interaction onto the renormalization of the electronic structure and the phonon-limited electronic transport properties for two prototypical TMD's: TaS_2 and WS_2. Our analysis and conclusions will be drawn closely to recent experimental findings [3].

[1] F. A. Rasmussen and K. S. Thygesen. Journ. of Phys. Chem. C **13** 169 (2015) [2] N. F. Hinsche *et al.*, ACS Nano **9** 4406 (2015) [3] C. E. Sanders *et al.*, Physical Rev. B. **94** 081404 (2016)

TT 26.5 Tue 10:30 POT 51

Spin Degenerate Regimes for Single Two-Dimensional Quantum Dots on Transition Metal Dichalcogenide Monolayers —

•Matthew Brooks and Guido Burkard — Department of Physics, University of Konstanz, D-78464, Germany

Strong spin orbit coupling in transition metal dichalcogenides (TMDCs) monolayers results in spin resolvable band structures about the K (K') valleys such that the eigenbasis of a 2D quantum dot (QD) on a TMDC monolayer in zero field is described by the Kramers pairs $|+\rangle = |K' \uparrow\rangle, |K \downarrow\rangle$ and $|-\rangle = |K \uparrow\rangle, |K' \downarrow\rangle$. This coupling limits the usefulness of single TMDC QDs as qubits due to the inherent difficulty of generating superposition states of the valley degree of freedom. Possible regimes of spin degenerate states overcoming the spin orbit coupling in monolayer TMDC QDs are investigated in both zero field, where the spin and valley degrees of freedom become fourfold degenerate, and in some magnetic field, localised to the K' valley. Such regimes are shown to be achieved in MoS_2, where the spin orbit coupling is sufficiently low that the spin resolved conduction bands intersect at points about the K (K') valleys and as such may be exploited by selecting suitable critical dot radii.

TT 26.6 Tue 10:45 POT 51

Electron Spin Relaxation in a Transition-Metal Dichalcogenide Quantum Dot — •Alexander Pearce and Guido Burkard — University of Konstanz, Konstanz, Germany

We study the relaxation of a single electron spin in a circular quantum dot in a transition-metal dichalcogenide monolayer defined by electrostatic gating. Transition-metal dichalcogenides provide an interesting and promising arena for quantum dot nano-structures due to combination of spin-valley physics and strong spin-orbit coupling. First we will discuss which bound state solutions in different B-field regimes can be used as the basis for qubits, at low B-fields combined spin-valley Kramers qubits and at large B-fields spin qubits. Then we will discuss the relaxation of a single electron spin mediated by electron-phonon interaction via various different relaxation channels. Rashba spin-orbit admixture mechanisms allow for relaxation by in-plane phonons arising either from the deformation potential or by piezoelectric coupling, additionally direct spin-phonon mechanisms involving out-of-plane phonons allow for relaxation. We find that the relaxation rates scale as $\propto B^4$ and $\propto B^2$ for in-plane phonons coupling via deformation potential and piezoelectric coupling respectively, while relaxation due to the direct spin-phonon coupling scales as $\propto B^2$. In the low B-field regime we also discuss the role of impurity mediated spin relaxation which will arise in disordered quantum dots.

Coffee Break

Invited Talk TT 26.7 Tue 11:30 POT 51

Influence of dark states on excitonic spectra of transition metal dichalcogenides — •Malte Selig[1,2], Dominik Christiansen[1], Gunnar Berghäuser[1,2], Ermin Malic[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden

In monolayers of transition metal dichalcogenides, excitonic effects play a significant role: Besides bright excitons, dark exciton states are formed by electrons and holes with opposite spin or constitute excitons with non-vanishing center of mass momentum well above the lightcone. Evaluating the excitonic states it turns out, that in tungsten based materials some of these dark states are energetically located below the optical accessible ones. Here, we develope excitonic Bloch equations for excitonic polarizations and densities under the influence exciton phonon interaction, adressing the strong impact of low lying dark states. We investigate the dephasing of the excitonic polarization through exciton phonon scattering [1] and the phonon mediated formation and thermalization of exciton densities. It turns out that coupling to low lying dark states is crucial for luminescence yield and lifetime. The presented results can explain several recent experimental results.

[1] M. Selig et al.,Nature Commun. 7,13279 (2016)

TT 26.8 Tue 12:00 POT 51

Transport measurements in graphene-WSe_2 heterostructures — •Tobias Völkl[1], Tobias Rockinger[1], Martin Drienovsky[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Universität Regensburg, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

Bringing graphene into proximity to WSe_2 was proposed as a way to induce a high spin orbit coupling strength in graphene, while maintaining the high intrinsic mobility of graphene. We therefore investigated the transport properties of graphene-WSe_2 heterostructures.

Placing graphene onto a WSe_2-flake resulted in mobilities around 10000 cm^2/Vs of graphene. Further a weak antilocalization behavior was observed, which indicates a high spin orbit coupling strength induced by the WSe_2.

Higher mobilities around 100000 cm^2/Vs were achieved by encapsulation of graphene between WSe_2 and hBN. In these samples no weak antilocalization behavior could be observed. We attribute this to a transition from diffusive to the quasiballistic regime. Also a feature dependent on the sample width arises in the low magnetic field range. We attribute this to a magneto size effect which further indicates quasiballistic behavior.

TT 26.9 Tue 12:15 POT 51

Electrical behavior of the oxidation of atomically thin $HfSe_2$ under ambient conditions — •Christopher Belke, Hennrik Schmidt, Benedikt Brechtken, Johannes C. Rode, Dmitri Smirnov, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover

12 years after the discovery of graphene [1], two-dimensional materials are of rising importance in the research and development section. An example for those layered materials are TransitionMetalDichalcogenide (TMD) with the chemical formula MX_2 , where M is a transition metal and X a chalcogenide [2]. Some materials are very fragile in ambient conditions. One of them is the n-type semiconductor hafnium diselenide ($HfSe_2$) [3]. During the fabrication the samples were prepared under nitrogen atmosphere or were covered with PMMA. An increasing resistance was measured while the sample was oxidized under ambient conditions, as well as a change of the electric field effect was observed.

[1] A. K. Geim et al., Nature Materials, **6**, 183 (2007)
[2] A. K. Geim, and I. V. Grigorieva, Nature **499**, 419 (2013)
[3] M. Kang et al. APL **106**, 143108 (2015)

TT 26.10 Tue 12:30 POT 51

ab initio **study of the transport properties in bulk and monolayer MX_3 (M = Ti, Zr, Hf and X = S, Se) compounds.** — •Yasir Saeed — Qatar Environment and Energy Research Institute (QEERI), Hamad Bin Khalifa University (HBKU), Qatar Foundation, P.O. Box 5825, Doha, Qatar

Two dimensional (2D) materials are best candidates for thermoelectric application due to their low thermal conductivity which is key property to achieve high efficiency for their usage in the filed of energy harvesting. Owing to that, here we present a study on electronic as well as thermal transport of bulk and monolayer MX_3 compounds (M = Ti, Zr, and Hf and X = S and Se) are investigated by by density functional theory and semi-classical Boltzmann theory. The bandgap amounts to rather similar value for bulk and monolayer, only the shape of band near Fermi level changes slightly, which results in a modified effective mass. We found that monolayer MX_3 compounds are good TE materials than bulk. Also p-type monolayer TiS_3 has twice large PF at 600 K than its room temperature value. However, monolayer $Zr/HfSe_3$ compounds showing promising behavior as a n-type TE materials at elevated high temperature of 600 K. In-plane tensile strain is also possible to tune the bandgap to increase S and disorder the monolayer lattice to minimize κ, therefore turns out to be a highly efficient approach for creating high performance TE materials.

TT 26.11 Tue 12:45 POT 51

Nonlinear Hall voltage from magnetic hot-spots — •Karina A. Guerrero Becerra, Andrea Tomadin, Andrea Toma, Remo Proietti Zaccaria, Francesco De Angelis, and Marco Polini — Istituto Italiano di Tecnologia, via Morego 30, I-16163 Genova, Italy

Electromagnetic simulations have recently shown that specifically designed plasmonic nanostructures are able to enhance and localize an oscillating magnetic field within a micro-meter area. These magnetic hot-spots, generated by forcing the plasmonic resonances of planar nanostructures to generate displacement currents of coil-type shape, have been shown to operate in the NIR [A. Nazir, *et. al.* Nano. Lett., 14, 3166-3171 (2014)] and in the MIR [S. Panaro, *et. al.* Nano. Lett., 15, 6128-6134 (2015)] frequency regions. Operating frequencies can be extended towards the THz regime. Here we propose that magnetic hot-spots might be probed through transport measurements by exploiting the response of the 2D electron gas (2DEG) hosted in a graphene bar, placed within the hot-spot area. We study the response

of the 2DEG, being subject to the oscillating in-plane electric field of the radiation driving the coil-type resonance, and to the localized magnetic field induced by it. We found that the response of the graphene 2DEG drives a rectification effect giving rise to a measurable Hall-like dc voltage, being sensitive to the operational frequency of the hot-spot. We discuss the conditions under which the predicted dc voltage is experimentally accessible, within the range of frequencies from THz to MIR. We show that the electric and magnetic fields within the hot-spot launch graphene plasma waves.

TT 26.12 Tue 13:00 POT 51

Exchange Interaction for Quantum Dots in TMDCs — •Alessandro David, Andor Kormanyos, and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We study the properties of double quantum dots in Transition Metal Dichalcogenides (TMDCs) where trapped electrons comprise not only the usual spin and valley degrees of freedom, but also a spin-orbit splitting in the spectrum. The spin-orbit coupling splits the four-fold spin and valley degeneracy into two Kramers pairs with correlated spin and valley states. We consider two different situations where the spin-orbit splitting is either much larger or comparable to the tunneling. Our aim is to use such systems filled with only two electrons for quantum information processing. In the case of large spin-orbit splitting, it turns out that there is a fourfold degenerate ground state (well separated from higher states) where, with a simple redefinition of Pauli matrices, we can obtain a CNOT gate in the same way it was obtained in the quantum computer proposed by Loss and DiVincenzo. In the case of small spin-orbit splitting, we have to consider a 16 dimensional subspace, but it is still possible to obtain a unitary evolution operator, that also depends on the value of spin-orbit splitting.

TT 27: Focus Session: Topological Insulators on Coupled Quantum Wells (joint session DS, HL, MA, O, TT, organized by HL)

Time: Tuesday 9:30–12:45 Location: POT 151

Invited Talk TT 27.1 Tue 9:30 POT 151

Edge conduction in the 2D topological insulator candidate InAs/GaSb — •Susanne Mueller, Matija Karalic, Christopher Mittag, Lars Tiemann, Thomas Tschirky, Quansheng Wu, Alexey A. Soluyanov, Atin Nath Pal, Christophe Charpentier, Matthias Troyer, Werner Wegscheider, Klaus Ensslin, and Thomas Ihn — Physics Department ETH Zurich, 8093 Zurich, Switzerland

We have studied transport measurements in mesoscopic Hall bars in the electrically tunable double quantum well structure InAs/GaSb. Helical edge states are predicted to dominate transport in the hybridization gap at zero magnetic field. We measure the non-local resistances and find a scaling according to Landauer-Büttikers expectations for helical edge modes [1]. No dependence on edge length could be observed in these devices, despite recent findings of trivial edges in this material system [2, 3]. To deepen the discussion, we are currently investigating the edge length dependence over a broader range of sample sizes and complete the discussion with clear experimental signature for the inverted phase [4] and the effect of strain on the bulk band structure [5], having in mind that an optimized bulk insulator is a necessary starting point for an edge study.

[1] S. Mueller et al., Phys. Rev. B 92, 081303 (2015)
[2] F. Nichele et al., New J. Phys. 18, 083005 (2016)
[3] B.-M. Nguyen et al., Phys. Rev. Lett. 117, 077701 (2016)
[4] M. Karalic, S. Mueller et al., Phys. Rev. B 94, 241402 (2016)
[5] L. Tiemann, S. Mueller et al., arXiv: 1610.06776

TT 27.2 Tue 10:00 POT 151

Topological Dirac Semimetals in GeSbTe vdW Heterostructures — •Peter Schmitz[1,3], Wei Zhang[2], Yuriy Mokrousov[3], and Riccardo Mazzarello[1] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen — [2]CAMP Nano, Xi'an Jiaotong University, China — [3]IAS-1 and JARA, Forschungszentrum Jülich

We investigate the spectral and topological properties of hexagonal TeSb[Te(GeTe)$_n$]SbTe van-der-Waals (vdW) heterostructures (GST-KH) as a function of strain, GeTe content and spin-orbit coupling (SOC) using density functional theory. We show that C_{3v} rotation symmetry stabilizes a massive 3D topological Dirac semimetal (TDSM) phase [1] in the entire family, thus going beyond previous topological insulator (TI) + normal insulator (NI) superlattice (SL) models [2]. The TDSM bulk Dirac cones move along k_z, proportional to the SOC profile and hybridization balance of corresponding interface states that gives rise to emergent magnetic gauge fields. The avoided crossings naturally allow perturbative hopping to build a tunable TDSM-heterostructure model and to include the c_S protected massive TDSM phase into the SL TI-to-NI transition as an expanded onset of the critical point where TDSM and 3D TI features merge. We attribute the TDSM dispersion of GST-KH to the internal $X(\mathrm{AX})_n$ film between polarizing SbTe caps and thereby create a link to generalized AX_2. To our knowledge, this is the first example of a (massive) TDSM in a vdW superlattice [*].

[*] doi.org/10.13140/RG.2.2.15113.85606

[1] B. Yang and N. Nagaosa, Nature Commun. 5, 4898 (2014)
[2] J. Tominaga et al, Adv. Mat. Inter. 1, 1300027 (2014)

TT 27.3 Tue 10:15 POT 151

Fractional quantum Hall effect in the $N = 2$ Landau level in bilayer graphene — Georgi Diankov[1], •Chi-Te Liang[1,2], François Amet[3,4], Patrick Gallagher[1], Menyoung Lee[1], Andrew Bestwick[1], Kevin Tharratt[1], William Coniglio[5], Jan Jaroszynski[5], Kenji Watanabe[6], Takashi Taniguchi[6], and David Goldhaber-Gordon[1] — [1]Department of Physics, Stanford University, Stanford, California 94305, USA — [2]Department of Physics, National Taiwan University, Taipei 106, Taiwan — [3]Department of Physics, Duke University, Durham, North Carolina 27708, USA — [4]Department of Physics and Astronomy, Appalachian State University, Boone, NC 28608, USA — [5]National High Magnetic Field Laboratory, Tallahassee, Florida 32310, USA — [6]Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305, Japan

To date, most fractional quantum Hall (FQH) studies have focused on the $N = 0$ lowest Landau level (LL). Here we report transport measurements of FQH states in the $N = 2$ LL (filling factors $4 < |\nu| < 8$) in bilayer graphene, a system with spin and valley degrees of freedom in all LLs, and an additional orbital degeneracy in the 8-fold degenerate $N = 0/N = 1$ LLs. In contrast with recent observations of particle-hole asymmetry in the $N = 0/N = 1$ LLs of bilayer graphene. The particle-hole symmetric FQH states in the $N = 2$ LL display energy gaps of a few Kelvin, comparable to and in some cases larger than those of fractional states in the $N = 0/N = 1$ LLs.

Invited Talk TT 27.4 Tue 10:30 POT 151

Progress in Edge Channel Transport of Two-Dimensional Topological Insulators — •Hartmut Buhmann — Physikalisches Institut, EP3, Universität Würzburg, Würzburg, Germany

The discovery of the quantum spin Hall (QSH) effect is already ten years old. However, an undisturbed edge channel transport has rarely been reported especially for samples which exceed a few micrometers in size, even though the QSH-states are protected against backscattering by time reversal symmetry. The reasons are manifold but mainly due to the fact that two-dimensional topological insulators are based on narrow gap semiconductors. Small disturbances and inhomogeneity may already result in potential fluctuations which introduce locally metallic electron or hole puddles. Edge channels traversing such puddles are no longer protected and backscattering destroys the expected perfect quantized conductance.

In this presentation I will review the experimental observations on two-dimensional topological insulators and give examples of how one can achieve almost perfect quantization in narrow gap samples. Taking special care during the fabrication process and taking advantage of charge accumulation at certain interfaces of the sample layer stack it becomes possible to observe quantized edge channel conductance even in sample exceeding the elastic mean free path. With these samples it is now possible to address various still open questions on the spe-

cific properties of the transport in helical edge channel as for example aspects of the magnetic field and temperature dependence.

Coffee Break

Invited Talk TT 27.5 Tue 11:30 POT 151

Transport and capacitance in HgTe-based topological insulators — •Dieter Weiss — Universität Regensburg, D-93040 Regensburg, Germany

The discovery of 2D and 3D topological insulators (TI) has opened an exciting area of condensed matter physics. It has been theoretically predicted and recently shown experimentally [1-3] that strained HgTe films constitute a 3D TI with a high-mobility 2D-electron gas enclosing the insulating bulk of HgTe. Here, I will show both transport and capacitance data obtained from different metal-oxide HgTe devices. Using top gates we can tune the gate voltage and thus explore quantum transport and quantum capacitance at different positions of the Fermi level E_F. Experiments on mesoscopic structures like nanowires and antidot superlattices made from strained 3D-HgTe films provide further evidence of the peculiar nature of topological surface states.

Work done in collaboration with D. A. Kozlov, D. Bauer, J. Ziegler, H. Maier, R. Fischer, S. Weishäupl, Z. D. Kvon, N. N. Mikhailov, and S. A. Dvoretsky

[1] C. Brüne et al., Phys. Rev. Lett. **106**, 126803 (2011)
[2] D. A. Kozlov et al., Phys. Rev. Lett. **112**, 196801 (2014)
[3] D. A. Kozlov et al., Phys. Rev. Lett. **116**, 166802 (2016)

TT 27.6 Tue 12:00 POT 151

Gate-tunable spin-charge conversion in single-layer graphene — •Masashi Shiraishi[1], Sergey Dushenko[1], Yuichiro Ando[1], Hiroki Ago[2], Taishi Takenobu[3], Susumu Kuwabata[4], and Teruya Shinjo[1] — [1]Kyoto University, Japan — [2]Kyushu University, Japan — [3]Nagoya University, Japan — [4]Osaka University, Japan

The small spin-orbit interaction of carbon atoms in graphene promises a long spin diffusion length and the potential to create a spin field-effect transistor. However, for this reason, graphene was largely overlooked as a possible spin-charge conversion material. In this presentation, an electric gate tuning of the spin-charge conversion voltage signal in single-layer graphene is reported [1]. Using spin pumping from an yttrium iron garnet ferrimagnetic insulator and ionic liquid top gate, we determined that the inverse spin Hall effect is the dominant spin-charge conversion mechanism in single-layer graphene. From the gate dependence of the electromotive force we showed the dominance of the intrinsic over Rashba spin-orbit interaction, a long- standing question in graphene research. Our study shows a simple spatial inversion symmetry breaking is not sufficient for generating the inverse Rashba-Edelstein effect, which is contrary to a conclusion in the other study [2].

References: [1] S. Dushenko, M. Shiraishi et al., Phys. Rev. Lett. 116, 166102 (2016). [2] J.B.S. Mendes et al., Phys. Rev. Lett. 115, 226601 (2015).

Invited Talk TT 27.7 Tue 12:15 POT 151

Giant Spin-Orbit Splitting in Inverted InAs/GaSb Double Quantum Wells — •Fabrizio Nichele[1], Morten Kjaergaard[1], Henri J. Suominen[1], Rafal Skolasinski[2], Michael Wimmer[2], Binh-Minh Nguyen[3], Andrey A. Kiselev[3], Wei Yi[3], Marko Sokolich[3], Michael J. Manfra[4], Fanming Qu[2], Arjan J. A. Beukman[2], Leo P. Kouwenhoven[2], and Charles M. Marcus[1] — [1]Center for Quantum Devices and Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen, Denmark — [2]QuTech, Delft University of Technology, 2600 GA Delft, The Netherlands — [3]HRL Laboratories, 3011 Malibu Canyon Road, Malibu, California 90265, USA — [4]Department of Physics and Astronomy and Station Q Purdue, Purdue University, West Lafayette, Indiana 47907 USA

We present transport measurements and numerical simulations that reveal a giant spin-orbit splitting of the bands in inverted InAs/GaSb quantum wells close to the hybridization gap. The splitting results from the interplay of electron-hole mixing and spin-orbit coupling, and can be larger than the hybridization gap. We experimentally investigate the band splitting as a function of top gate voltage for both electronlike and holelike states. Unlike conventional, noninverted two-dimensional electron gases, the Fermi energy in InAs/GaSb can cross a single spin-resolved band, resulting in full spin-orbit polarization. In the fully polarized regime we observe exotic transport phenomena such as quantum Hall plateaus evolving in e^2/h steps and a nontrivial Berry phase.

TT 28: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - III (joint session DS, HL, MA, MM, O, TT, organized by O)

Time: Tuesday 10:30–13:00 Location: GER 38

Invited Talk TT 28.1 Tue 10:30 GER 38

Including spin effects in the strong-coupling limit of DFT — •Paola Gori-Giorgi[1], Juri Grossi[1], Derk Pieter Kooi[1], Klaas Giesbertz[1], Michael Seidl[1], Aron Cohen[2], and Paula Mori-Sanchez[3] — [1]Vrije Universiteit Amsterdam, The Netherlands — [2]University of Cambridge, UK — [3]Universidad Autonoma de Madrid, Spain

The exact strong-coupling limit of density functional theory (DFT) reveals a different mathematical structure with respect to the one of traditional approximations for the exchange-correlation (xc) functional: instead of the local density, local density gradients, or quantities related to the Kohn-Sham orbitals, some integrals of the density appear in this limit. In the recent years, xc functionals directly inspired to this mathematical structure have been constructed and implemented in an efficient way. However, the leading terms (exact or approximate) in the strong-coupling limit of DFT are intrinsically semiclassical and, as such, do not incorporated the spin dependence. In this talk, I will present the first study on the incorporation of the spin-dependence in the exact strong-coupling limit in simple one-dimensional cases. I will then discuss approximations for our findings and routes to the construction of spin-dependent xc functionals for strong coupling. Comparison with exact calculations for the Hohenberg-Kohn functional in the strong-coupling regime confirms the accuracy of our expressions for the leading terms.

TT 28.2 Tue 11:00 GER 38

Strong correlation from the Random Phase Approximation and beyond — •Thomas Olsen and Kristian Thygesen — Department of Physics, Technical University of Denmark

We assess the performance of the Random Phase Approximation (RPA) for strongly correlated systems and discuss different routes to venture beyond RPA. It is well-known that RPA reproduces the dissociation curve of molecular H2 correctly and thus accurately captures the strong static correlation inherent in the dissociation limit. It is thus natural to ask whether RPA is able to describe the strongly correlated Mott insulators as well. In particular, the accurate description of antiferromagnetic systems is complicated by the fact that the magnetic order often emerges from a detailed interplay between direct exchange and super-exchange couplings, which are respectively exchange and correlation effects. Whereas DFT+U, semi-local and hybrid functionals are often capable of describing either exchange or super-exchange accurately, RPA is shown to give an accurate account of both. We will finally show that RPA can be improved by either including non-local kernel in the framework of TDDFT or including electron-hole interactions in the irreducible response function. Only the latter approach improves the description of strong correlation, whereas the former approach improves atomization energies significantly compared to RPA.

TT 28.3 Tue 11:15 GER 38

Surface and adsorption energy calculations within the random phase approximation — •Per Schmidt and Kristian Thygesen — Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The application of density functional theory (DFT) to the calculation of adsorption and surface energies is ever increasing and as a theory,

it has the potential to e.g. guide experiments in the search of better catalysts. However, a previous study[1] shows that with standardly used semi-local functionals, DFT is not able to accurately predict surface and adsorption energies simultaneously. By tuning the functional, either the predicted surface or adsorption energies can be improved at the expense of the other. For a few cases however, it has been shown[1] that the many-body approach, the random phase approximation (RPA), yields both excellent surface and adsorption energies.

In this work we expand the use of the RPA method to eight adsorption reactions over 20 transition metal surfaces using the electronic structure code GPAW. We report the difference in surface and adsorption energies compared with the standard DFT functionals: PBE, RPBE and BEEF-vdW. We find that RPA does in general predict less stable surfaces, in better agreement with experiments and the average change in adsorption energies varies between ± 0.5 eV. The RPA values could be used to guide construction of new density-functionals aimed at improving surface science calculations.

[1] L. Schimka, J. Harl, A. Stroppa, A. Grüneis, M. Marsman, F. Mittendorfer, and G. Kresse, Nature Materials 9, 741 (2010).

TT 28.4 Tue 11:30 GER 38

Large-scale cubic-scaling RPA correlation energy calculations using a Gaussian basis — •Jan Wilhelm and Jürg Hutter — University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

The random phase approximation (RPA) for computing the electron correlation energy has emerged as an accurate tool for predicting the properties of molecules and condensed phase systems. RPA combines a number of attractive features, most importantly that long-range van der Waals interaction is included, in contrast to semilocal density functionals. The drawback connected with RPA is the computational cost: For canonical implementations of RPA, the numerical effort grows as quickly as $O(N^4)$ with the system size N. We present an algorithm for computing the RPA correlation energy in a Gaussian basis requiring $O(N^3)$ operations and $O(N^2)$ memory. The cubic-scaling RPA method is based on the resolution of the identity (RI) with the overlap metric, a reformulation of RI-RPA in the Gaussian basis and imaginary time as well as the use of sparse linear algebra. We report a massively parallel implementation which is the key for the application to large systems. As first benchmark of the method, we show the RPA correlation energy of thousands of water molecules in a high-quality cc-TZVP basis. For a comparison, the canonical RPA method is restricted to 500 water molecules using the whole Piz Daint supercomputer for two hours. Our RPA algorithm enables the application of RPA to large systems where van der Waals interactions play an important role, e.g. for predicting the adsorption energy of large molecules on surfaces.

TT 28.5 Tue 11:45 GER 38

Semi-local exchange functionals showing ultranonlocal response: the hope to replace exact exchange — •Thilo Aschebrock and Stephan Kümmel — Theoretical Physics IV, University of Bayreuth, D-95440 Bayreuth, Germany

The widespread success of Density Functional Theory (DFT) is based on a favorable ratio of accuracy to computional cost, especially with semi-local approximations to the exchange-correlation energy. However, functionals such as the local density approximation (LDA), generalized-gradient approximations (GGA) or meta-generalized-gradient approximations (meta-GGA), typically miss important exact exchange features related to the derivative discontinuity. These are essential for accurately describing long-range charge transfer processes. The electrical response of molecular chains, which is dramatically overestimated by local and semi-local density functionals, is a prime example. The key to its correct description is a term in the Kohn-Sham exchange potential that counteracts the external field and has been named "ultranonlocal". We here present how these field-counteracting properties can be incorporated into semi-local DFT on the meta-GGA level. Thereby we show that by utilizing the kinetic-energy-density, it is possible to model ultranonlocal effects in the Kohn-Sham potential by virtue of a semi-local energy expression.

TT 28.6 Tue 12:00 GER 38

(De)stabilizing dispersion interactions via external electric charges — •Andrii Kleshchonok[1] and Alexandre Tkatchenko[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg

Van der Waals (vdW) or dispersion interactions play a central role in the structure, stability, and reaction mechanisms in large variety of molecules and materials. However, in many situations of interest in material science and biophysics, vdW interactions should account for the coupling with external (in)homogeneous electric fields. In this work we address the effect of external static charge field on long-range electron correlations. By using the quantum Drude oscillator model, we derive analytical expressions of the charge induced dipole-quadrupole dispersion energy, that is accounted neither in standard DFT methods, nor in popular vdW correction schemes. Analysing the scaling laws of this dispersion term, we conclude that positive charge stabilizes dispersion interactions, while a negative charge has an opposite effect. Benchmark over S22 molecular dataset estimates the induced dispersion to be in the range of 20-300 % of conventional electrostatic energy. Our findings could have broad potential implications, including exfoliation of 2D materials, chemical reaction rates in charged droplets, and biological membranes.

TT 28.7 Tue 12:15 GER 38

An optimisability proof for self-consistent constrained DFT, and its implications for constraint-based self-interaction error correction — Glenn Moynihan[1], Gilberto Teobaldi[2,3], and •David D. O'Regan[1] — [1]School of Physics, CRANN and AMBER, Trinity College Dublin, Ireland. — [2]Stephenson Institute for Renewable Energy and Department of Chemistry, The University of Liverpool, U.K. — [3]Beijing Computational Science Research Center, China.

We develop the connection between constrained DFT energy derivatives and response functions, providing a rigorous assessment of the uniqueness and character of cDFT stationary points while accounting for electronic interactions and screening [1]. In particular, we provide a non-perturbative proof that stable stationary points of linear density constraints occur only at energy maxima with respect to their Lagrange multipliers, generalizing the proof of Ref. [2]. We demonstrate that multiple solutions, hysteresis, and energy discontinuities may occur in cDFT, and we provide necessary conditions for the optimizability of multi-constraint cDFT. We show that the applicability of cDFT in automating symmetry-preserving self-interaction error corrections is limited by a fundamental incompatibility with non-linear constraints. We circumvent this by utilizing separate linear and quadratic correction terms, which may be interpreted either as distinct constraints, each with its own Hubbard U type Lagrange multiplier, or as the components of a generalized, two-parameter DFT+U functional [3]. [1] Phys. Rev. B **94**, 035159 (2016). [2] Phys. Rev. A **72**, 024502 (2005). [3] Phys. Rev. B Rapid Comms., Accepted (2016), arXiv:1608.07320.

TT 28.8 Tue 12:30 GER 38

Density-based local hybrid functional for interfaces — •Pedro Borlido[1], Silvana Botti[1], and Miguel Marques[2] — [1]Institu für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743, Jena, Germany — [2]Instiut für Physik, Martin-Luther-Universität Halle Wittenberg, D-06099 Halle, Germany

Hybrid functionals in density functional theory have become the state-of-the-art for the calculation of electronic properties of solids. The key to their performance is how and in which amount a part of Fock exchange is mixed with semi-local exchange-correlation functionals. We propose here a material dependent and local mixing parameter which is a functional of the electron density alone, through an estimator of the local dielectric function inspired by the work done in *Phys. Rev. B* 83, 035119 (2011). This new functional is by construction an approximation of the *GW* self-energy and it enables therefore calculations of quasiparticle energy levels of comparable quality as *GW*, but at the reduced cost of a hybrid density functional. In contrast with other recent self-consistent schemes for the mixing parameter, our approach does not require to calculate the dielectric function and leads to a negligible increase of the computation time.

TT 28.9 Tue 12:45 GER 38

On the hunt for better functionals in DFT: a new quantum embedding scheme — •Uliana Mordovina[1], Teresa E. Reinhard[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

We propose a new systematic technique to derive functionals for standard density functional theory (DFT) in an ab-initio fashion. This technique origins in the recently developed density-matrix embedding

theory (DMET) [1]. DMET is a quantum-in-quantum embedding method, which is based on finding a projection between the high-dimensional wave function of the full system and a lower-dimensional wavefunction living in the active space of the embedded system, which is then solved exactly. In the original DMET scope, the projection is improved via optimization of the reduced one-body density matrix. We replace this optimization by a density inversion, exploiting the one-to-one mapping between electronic density and Kohn-Sham potential.

Not only the DMET scheme is improved by the uniqueness of the density-potential mapping, the proposed density-embedding also allows for finding accurate Kohn-Sham potentials. Moreover, unlike in usual DFT, we can systematically improve the description by increasing the size of the active space.

We show benchmark results of our method for molecules in 1D.

[1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012)

TT 29: Other Low Temperature Topics: Cold Atomic Gases

Time: Tuesday 12:00–13:00 Location: HSZ 201

TT 29.1 Tue 12:00 HSZ 201

Universal upper bound on the condensate-concentration of lattice hard-core bosons — Felix Tennie[1], Vlatko Vedral[1,2], and •Christian Schilling[1] — [1]Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom — [2]Centre for Quantum Technologies, National University of Singapore, 3 Science Drive 2, Singapore 117543

To investigate Bose-Einstein condensation for interacting bosons, usually the largest eigenvalue of their one-particle reduced density matrix is calculated. For lattice systems of N hard-core bosons on d sites we take a complementary viewpoint: Independent of the spatial dimension and any further microscopic details we prove that the hard-core constraint enforces a universal upper bound on occupation numbers given by $N_{max} = (N/d)(d - N + 1)$. It can only be attained for one-particle states $|\varphi\rangle$ with equal amplitudes with respect to the hard-core basis (sites) and when the corresponding N-particle state $|\Psi\rangle$ is maximally delocalized. We show that the maximizing state $|\Psi\rangle$ is related to the ground state of a bosonic 'Hubbard star' showing Bose-Einstein condensation.

TT 29.2 Tue 12:15 HSZ 201

Quasiparticle-induced Damping of BEC Oscillations in Double-well Potentials — •Tim Lappe[1], Anna Posazhennikova[2], and Johann Kroha[1] — [1]Physikalisches Institut, Universität Bonn — [2]Department of Physics, Royal Holloway, University of London

An interacting Bose-Einstein condensate (BEC) in a double-well trap with initial population imbalance, z_0, can perform Josephson oscillations or be in a self-trapped regime, depending on the value of z_0. Experimentally, both strongly damped [1] and undamped Josephson oscillations [2] have been observed, a discrepancy that has remained controversial because the source of the damping in [1] could not be clearly identified. A known mechanism for damping in such systems is via inelastic collisions of quasiparticles (QPs) [3]. However, in order to compare with real experiments one needs to incorporate the realistic energy spectrum of the potential, temperature effects and condensate contributions to the higher excited levels of the trap. In view of the necessary changes we solve the full non-separable potential of [2] exactly and incorporate all fluctuation effects within the full second order (in the couplings) approximation, thus demonstrating the possibility of QP excitations in the system. By taking into account QP collisions, we can reproduce the damped oscillations.

[1] LeBlanc et. al., Phys. Rev. Lett. **106**, 025302 (2011).
[2] Albiez et. al., Phys. Rev. Lett. **95**, 010402 (2005).
[3] A. Posazhennikova, M.Trujillo-Martinez, J. Kroha, Phys. Rev. Lett. 116, 225304 (2016).

TT 29.3 Tue 12:30 HSZ 201

Synthetic Creutz-Hubbard Model: Interacting Topological Insulators with Ultracold Atoms — Johannes Jünemann[1,2], Angelo Piga[3], Shi-Ju Ran[3], Maciej Lewenstein[3,4], •Matteo Rizzi[1], and Alejandro Bermudez[5,6] — [1]Johannes Gutenberg-Universität, Mainz (Germany) — [2]MAINZ - Graduate School Materials Science in Mainz (Germany) — [3]ICFO-Institut de Ciencies Fotoniques, Castelldefels (Spain) — [4]ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona (Spain) — [5]Swansea University (UK) — [6]Instituto de Física Fundamental, IFF-CSIC, Madrid (Spain)

Understanding the robustness of topological phases of matter in the presence of strong interactions, and synthesising novel strongly-correlated topological materials, lie among the most important challenges of modern theoretical and experimental physics. Here we present a complete theoretical analysis of the Creutz-Hubbard ladder, a paradigmatic model that provides a neat playground to address these challenges. We put special attention to the competition of exotic topological phases and orbital quantum magnetism in the regime of strong interactions and identify the universality class of the different phase transitions. These results are furthermore confirmed and extended by extensive numerical simulations and analysis of the entanglement properties. Moreover, we propose how to experimentally realize this model and test its phase diagram in a synthetic ladder, made of two internal states of ultracold fermionic atoms in a one-dimensional optical lattice. Our work paves the way towards quantum simulators of interacting topological insulators with cold atoms.

TT 29.4 Tue 12:45 HSZ 201

Full counting statistics with determinantal quantum Monte Carlo — •Stephan Humeniuk — Institute for Theoretical Physics III, University of Stuttgart

Within the framework of determinantal quantum Monte Carlo, a method is presented for computing the probability distribution of the total particle number and magnetization on a subregion of a system of interacting fermions. Such full counting statistics can be obtained from repeated projective measurements in cold atoms experiments with single-site and single-atom resolution. Applied to the attractive Hubbard model, the full counting statistics reveals the size of a preformed pair or Cooper pair as a function of interaction strength.

TT 30: Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Tuesday 14:00–16:00 Location: HSZ 03

TT 30.1 Tue 14:00 HSZ 03

Renormalized Perturbation Theory as a General Solver for Quantum Impurities — •Simon Jahns and Gertrud Zwicknagl — Institut für Mathematische Physik, TU Braunschweig, Germany

In systems with magnetic impurities conduction electrons are scattered by low energy spin fluctuations leading to the Kondo effect. Due to the strong local electron interactions the low energy scales can not be accessed perturbatively. However, here we are demonstrating the efficiency and flexibility of the RPT [1] as a gerneral impurity solving technique, with which this problem is circumvented.

The central idea is to first determine the renormalized quasiparticle characteristics and to subsequently calculate the Green's functions from a perturbation expansion in terms of the quasiparticle propagators and effective interactions.

The fully renormalized quasiparticle parameters are derived from flow equations connecting a (sometimes hypothetical) weak-coupling regime to the physically relevant strong-couping regime. Typical examples for the flow variable are an external magnetic field or the chemical potential. Results for the single impurity Anderson model (SIAM) have been found in excellent agreement with exact solutions [2].

We discuss the extension of the scheme to more general quantum impurity models accounting to e.g. for Hund's rule correlations.

[1] K. Edwards, A. C. Hewson, J. Phys.: Condens. Matter 23 (2011)
[2] K. Edwards, A. C. Hewson, V. Pandis, Phys. Rev. B 87 (2013)

TT 30.2 Tue 14:15 HSZ 03

Numerical Renormalization Group study of Gate Induced Kondo Screening in Graphene — •Daniel May[1], Jinhai Mao[2], Yuhang Jiang[2], Po-Wei Lo[3,4], Guohong Li[2], Guang-Yu Guo[3,4], Frithjof Anders[1], and Eva Y. Andrei[2] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik 2, Germany — [2]Rutgers University, Department of Physics and Astronomy, USA — [3]National Taiwan University, Department of Physics, Taiwan — [4]National Center for Theoretical Sciences, Physics Division, Taiwan

Graphene in its pristine form has transformed our understanding of 2D electron systems leading to fundamental discoveries. When graphene's honeycomb lattice is disrupted by single atom vacancies, new phenomena, namely a re-entrance Kondo effect, may emerge. We present numerical renormalization group (NRG) calculations for a two-orbital model consisting of a local σ orbital and a localized π state induced by the vacancy. Guided by ab-initio calculations for the parameters we determine two regimes. The re-entrance regime (i) is characterized by a conventional Kondo effect (p doping), a breakdown of the Kondo peak for vanishing chemical potential $|\mu| \to 0$, and a underscreened Kondo (n doped) where the π conduction band is screening the magnetic moment of the σ orbital. Increasing the hybridization between the σ orbital and the π conduction band further drives the system into the second regime (ii) where the π state is depopulated and a conventional Kondo effect is present (p doped).

TT 30.3 Tue 14:30 HSZ 03

Interplay of Superconductivity and Magnetism in the 2D Kondo Lattice Model: A Variational Cluster Approach — •Benjamin Lenz, Riccardo Gezzi, and Salvatore R. Manmana — Institute for Theoretical Physics, Georg-August-Universität Göttingen

We present results for the interplay of d-wave superconductivity and antiferromagnetism in the Kondo lattice model using the variational cluster approximation (VCA). Both the paramagnetic and the antiferromagnetic phase of the model are investigated and regions with different Fermi surface topology are found in the latter. The transition between these two different antiferromagnetic phases is investigated close to and off half-filling. VCA is used to probe the system for s-wave and d-wave superconductivity for all coupling regions. It is shown that only by treating antiferromagnetism and superconductivity on equal footing artificial superconducting solutions at half-filling can be avoided. No true s-wave superconducting solutions due to correlation effects are found, but d-wave pairing proves to be robust for various coupling strengths off half-filling. Its interplay with antiferromagnetism is analyzed at weak coupling.

TT 30.4 Tue 14:45 HSZ 03

Nonequilibrium Kondo effect in a magnetic field: Auxiliary master equation approach — •Delia Fugger[1], Frauke Schwarz[2], Antonius Dorda[1], Jan von Delft[2], Wolfgang von der Linden[1], and Enrico Arrigoni[1] — [1]Institute of Theoretical and Computational Physics, TU Graz, Austria — [2]Faculty of Physics, LMU Munich, Germany

We solve the single-impurity Anderson model in a magnetic field and out of equilibrium with an auxiliary master equation approach [1,2]. Employing Matrix Product States techniques to solve the many-body Lindblad equation allows us to generate highly accurate results, especially for the spectral functions. In equilibrium we find a remarkable agreement with spectral functions obtained with NRG, cf. [2].

The application of a bias voltage V and a magnetic field B both individually result in a splitting of the Kondo resonance around the Kondo temperature. With our method we can resolve a four-peak structure in the spectral function for nonzero B and V, due to both effects. This four-peak structure manifests itself in the differential conductance, which is very well accessible by experiments.

We investigate the stationary properties of the system as well as its dynamics after a quantum quench. We finally compare our results to recent experiments [3] and draw conclusions about the underlying spectral functions. We find that our results nicely agree with experimental data also outside the Kondo regime.

[1] E. Arrigoni et al., PRL 110, 086403 (2013)
[2] A. Dorda et al., PRB 92, 125145 (2015)
[3] A. V. Kretinin et al., PRB 84, 245316 (2011)

TT 30.5 Tue 15:00 HSZ 03

Topological protected quantum critical point in 1D Two Impurity Models — •Fabian Eickhoff, Benedikt Lechtenberg, and Frithjof Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44227 Dortmund

The two impurity Anderson model exhibit an additional quantum critical point at infinitely many specific distances between both impurities for an inversion symmetric 1D dispersion. Unlike the quantum critical point previously established by Jones and Varma, it is robust against particle-hole or parity symmetry breaking. The quantum critical point separates a spin doublet from a spin singlet ground state and is, therefore, topological protected. A finite single particle tunneling t or an applied uniform gate voltages will drive the system across the quantum critical point. The discriminative magnetic properties of the different phases cause a jump in the spectral functions at low temperature which might be useful for future spintronics devices. A local parity conservation will prevent the spin-spin correlation function to decay to its equilibrium value after spin-manipulations.

TT 30.6 Tue 15:15 HSZ 03

AFM mechanical dissipation due to onset of Kondo impurity screening — •Pier Paolo Baruselli, Michele Fabrizio, and Erio Tosatti — SISSA, Via Bonomea 265 34136 Trieste (Italy)

In nanomechanical systems such as STM tips approaching magnetic sites on a surfaces, some cases have been reported where the tip may cause the switching of the impurity spin from zero or one, to a spin 1/2 showing up as a Kondo conductance peak. Since at the same time one can in principle measure the tip mechanical dissipation, it is relevant to investigate theoretically what contribution will the onset of a Kondo state make to that dissipation. As a starting point we model the Kondo state as a non-interacting resonant level, showing that the dissipation, proportional to the Kondo energy, diverges roughly as the logarithm of the temperature. We then discuss extensions of our approach using an Anderson model solved by numerical renormalization group, which accounts for many-particle effects. We finally speculate about the role of a finite driving frequency.

Sponsored by ERC MODPHYSFRICT Advanced Grant No. 320796

TT 30.7 Tue 15:30 HSZ 03

The spinless Anderson-Holstein impurity model — •Andisheh Khedri[1,2], Volker Meden[1,2], and Theo Costi[2] — [1]RWTH Aachen Univercity — [2]Forschungszentrum Jülich

We consider a spinless resonant level in a wide conduction band which is coupled to a phonon mode. This coupling induces an effective retarded and attractive electron-electron interaction which leads to a

suppression of the tunneling rate from the local level to the conduction sea. Conventional perturbation theory in the coupling strength does neither capture the underlying polaron physics nor the power-law like renormalization as known from the purely fermionic interacting resonant level model (anti-adiabatic limit). We use the functional renormalization group to study the renormalization of the tunneling rate for arbitrary bare rate and phonon frequency in the limit of small to intermediate electron-phonon coupling. We compare to results obtained by the numerical renormalization group.

TT 30.8 Tue 15:45 HSZ 03

A modified Anderson impurity model in a continuum limit of the Hubbard model — •Yahya Öz and Andreas Klümper — Bergische Universität Wuppertal

Starting from the integrable Hubbard model by use of the R-matrix a new model with impurity and modified dispersion relation is obtained. We consider the thermodynamical approach based on the well-known finite set of non-linear integral equations (NLIE) of convolution type for obtaining the integrable modification of the energy-momentum dispersion for the derivation of the thermodynamic equations of this new model. This integrable lattice model can be used for obtaining the Anderson impurity model in the continuum with a modified dispersion relation.

TT 31: Correlated Electrons: Other Materials

Time: Tuesday 14:00–16:00 Location: HSZ 103

TT 31.1 Tue 14:00 HSZ 103

Dipolar effects on the critical fluctuations in Fe: Investigation by MIEZE — •Steffen Säubert[1,2], Jonas Kindervater[3], and Peter Böni[1] — [1]Physik Department, Technische Universität München, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [3]Institute for Quantum Matter and Department of Physics and Astronomy, Johns Hopkins University, Baltimore, USA

Iron is one of the archetypical ferromagnets to study the critical fluctuations at a continuous phase transition thus serving as a model system for the application of scaling theory. We report a comprehensive study of the critical dynamics at the transition from the ferro- to the paramagnetic phase in Fe, employing the high-resolution neutron spin echo technique MIEZE. The results show that the dipolar interactions lead to an additional damping of the critical spin fluctuations at small momentum transfers $\mathbf{q}$. The results agree essentially with scaling theory if the dipolar interactions are taken into account by means of the mode-coupling equations. However, in contrast to expectations, the dipolar wavenumber q_D that plays a central role in the scaling function $f(\kappa/q, q_D/\kappa)$ becomes temperature dependent. In the limit of small $\mathbf{q}$ the critical exponent z crosses over from 2.5 to 2.0.

TT 31.2 Tue 14:15 HSZ 103

Electronic Structure of Palladium Determined by Compton Scattering and Electron-Positron Annihilation — •Josef Helmut Schmidbauer, Josef Andreas Weber, Michael Leitner, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany

Compton scattering and the measurement of the angular correlation of electron-positron annihilation radiation (ACAR) offer two complementary techniques for the investigation of the electronic structure of materials. We applied both methods to determine the bulk electron momentum distribution of the 4d transition element palladium. By reconstructing the full Fermi surface from 2D-ACAR projections we reveal all major features of the Fermi surface, predicted by theoretical calculations. Based on our experimental findings and by comparison with theory we discuss correlation effects in Palladium. Moreover, we examine the shape of the so-called L-hole pocket in order to compare the results of different theoretical calculation schemes.

TT 31.3 Tue 14:30 HSZ 103

Importance of Mott physics in manganese pnictides — •Manuel Zingl, Elias Assmann, and Markus Aichhorn — Institute of Theoretical Physics and Computational Physics, Graz University of Technology, Austria

Manganese pnictides, e.g. $BaMn_2As_2$ and LaMnAsO, attract attention due to their exceptional physical properties. Thus, revealing the underlying electronic mechanisms is highly desired. These compounds have a nominally half-filled d shell, and as a consequence, electronic correlations are strong, placing them at the verge of a metal-insulator transition. In addition to electronic correlations, the effective dimensionality is another fundamental factor in understanding their physical properties. We demonstrate that experimentally observed Néel temperatures, band gaps, conductivities and also Seebeck coefficients of the compounds under consideration can be explained by our DFT+DMFT calculations.

TT 31.4 Tue 14:45 HSZ 103

Quantum Oscillations in $CoSb_3$ — •Marcel Naumann[1], Frank Arnold[1], Flipo Sever[1], Mirtha Pillaca Quispe[2], Dan Sun[1], Michael Baenitz[1], Andreas Leithe-Jasper[1], Helge Rosner[1], Peter Gille[2], and Elena Hassinger[1,3] — [1]Max-Planck-Institut Chemische Physik fester Stoffe, Dresden, Germany — [2]Ludwig-Maximillians-Universität München, Germany — [3]Technische Universität München, Garching, Germany

The material class of skutterudites is at the center of attention on the search for new thermoelectric materials. Additionally, they also host a variety of novel electronic properties, such as valence fluctuations and non-fermi liquid behaviour, which are widely studied in condensed matter physics. The skutterudite $CoSb_3$, in particular, is a parent compound, whose doped and "filled" variants are studied in the aforementioned fields. It is characterised by two linearly dispersing bands, which anticross close to the Fermi level at the Γ-point, coexisting with a heavier electron band above the crossing.

Here we present a comprehensive experimental study of the bulk Fermi surface of $CoSb_3$. By means of quantum oscillations, measured in magnetisation and angle-dependent electronic transport, information about topology, charge carrier effective mass and scattering times are gained. Two Fermi surfaces of similar size are observed. Their size and topology fit the charge carrier density determined by Hall measurements and ab-initio DFT calculations for slight electron doping. Furthermore, we show reproducible doping levels and crystal quality throughout a variety of sample batches.

TT 31.5 Tue 15:00 HSZ 103

Unconventional superconductivity in unconventional correlated materials? — •Xiaodong Cao[1], Jean Chen[1], Zhicheng Zhong[1], Dirk Manske[1], Thomas Ayral[2], Olivier Parcollet[2], and Philipp Hansmann[1] — [1]Heisenbergstrasse 1,D-70569 Stuttgart, — [2]Institut de Physique Théorique (IPhT), CEA, CNRS, UMR 3681, 91191 Gif-sur-Yvette, France

Rare earth heavy fermion systems or transition metal oxides are probably among the first materials that come to mind when we consider unconventional superconductivity in strongly correlated materials. However, a much less known class of compounds, synthesized by the adsorption of a specific ad-atom species on a semiconductor substrate, have been recently confirmed as highly correlated systems. Depending on the specific ad-atom the materials span a rich variety of correlation physics including Mott insulating ground states or correlation driven charge order. With an effective Hamiltonian derived from ab initio methods, we adapt the dynamical-mean field theory, albeit including also non-local correlations on the level of the three legged electron boson vertex as recently proposed by Ayral and Parcollet. Studying the interplay of effects induced by long range interaction, geometric frustration, we started our search to novel exotic ground states. Interestingly, for the specific case of Pb/Si(111) preliminary results already suggest the presence of a d+id chiral superconductivity as a function of doping.

TT 31.6 Tue 15:15 HSZ 103

Electron spin resonance of the spin chain compound $Cu(py)_2Br_2$: An experimental and theoretical study — Julian Zeisner[1], Stephan Zimmermann[1], Vladislav Kataev[1], •Michael Brockmann[2], Frank Göhmann[2], Andreas Klümper[2], and Alexander Weisse[3] — [1]Leibnitz Insitute for Solid State and

Material Research, Dresden, Germany — [2]University of Wuppertal, Germany — [3]Max Planck Institute for Mathematics, Bonn, Germany

We analyze electron spin resonance (ESR) data of the quasi-one-dimensional magnet $Cu(py)_2Br_2$ and compare with theoretical predictions for the spin-1/2 Heisenberg chain with small anisotropic perturbations.

Based on measurements of the angular dependence of resonance shift and linewidth at high temperatures the full g-tensor can be determined and the existence of two anisotropy axes oriented perpendicular to the chain axes is proposed. We further estimate the strength of the anisotropy from several ESR data, in particular from the frequency dependence of the resonance shift at low temperatures, showing that usual field theoretical approaches at zero temperature are not sufficient to explain our low-temperature data. Furthermore, from the angular dependence of the linewidth, the algebraic decay of dynamical correlation functions of the isotropic spin chain can be deduced ($\sim t^{-2/3}$). This result does not agree with the picture of spin diffusion in one dimension ($\sim t^{-1/2}$).

TT 31.7 Tue 15:30 HSZ 103

Hydrodynamic transport in Anisotropic-Dirac Systems — •Julia Link[1], Boris Narozhny[1], and Jörg Schmalian[1,2] — [1]Institute for Theory of Condensed Matter (TKM), Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute for Solid State Physics (IFP), Karlsruhe Institute of Technology, Karlsruhe, Germany

We present the transport properties of anisotropic-Dirac fermion systems in the hydrodynamic regime. Anisotropic Dirac-fermions are new and interesting materials similar to graphene. These materials have a Fermi-Dirac point. However, the energy dispersion is linear along one axis and parabolic in the perpendicular direction. Thus the fermions behave relativistic in one direction and classical in the perpendicular direction. This leads to fascinating transport behavior. Studying one Fermi-point using the qunatum Boltzmann equation, we find insulating behavior in the relativistic regime and metallic behavior in the classical regime. We discuss the implications for TiO_2/VO_2 which is a square lattice and has two Fermi-Dirac points in one Brillouin zone, which are rotated by 90-degrees relative to each other. The conductivity is thus a superposition of the insulating and metallic behavior. In order to disentangle the relativistic and classical transport regimes, we study the magnetoresistivity.

TT 31.8 Tue 15:45 HSZ 103

Casimir forces between two impurities in a lattice — •Andrei Pavlov[1], Dmitri Efremov[1], and Jeroen van den Brink[1,2] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany — [2]Institute for Theoretical Physics, TU Dresden, 01069 Dresden, Germany

One of the fundamental properties of matter is the Casimir force, i.e. interaction of classical objects via quantum fluctuations. It appears in various field, including optics, Bose-condensates, micro-structure geometry compounds, etc. The usual wisdom is that the Casimir force between two atoms decays as $r^{-(2D+1)}$, which is originated from the two boson exchange in the lowest order of the perturbation theory. Stimulated by the recent experiments on the high temperature superconductor H_3S under high pressure, we reconsider the Casimir forces between two impurities in solid state physics via virtual phonons at long and short distances. We found strong deviation from the standard law at short distances which depends on the masses of impurities atoms. At long distances it comes to the standard r-dependence, but the value of the prefactor is much larger than it's expected from the lowest orders of the perturbation theory. These differences become important when the impurity masses differ from the lattice atoms more than twice. Finally we apply our results to impurity atoms of deuterium and tritium in H_3S.

TT 32: Transport: Nanomechanics and Optomechanics (jointly with CPP, DY, BP, DF)

Time: Tuesday 14:00–15:15 Location: HSZ 201

TT 32.1 Tue 14:00 HSZ 201

Classical Stückelberg interferometry of a nanomechanical two-mode system — •Maximilian Seitner[1,2], Hugo Ribeiro[3], Johannes Kölbl[1], Thomas Faust[2], Jörg Kotthaus[2], and Eva Weig[1,2] — [1]Departement of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Center for NanoScience (CeNS) and Fakultät für Physik, Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, München 80539, Germany — [3]Department of Physics, McGill University, Montreal, Quebec, H3A 2T8, Canada

Stückelberg interferometry is a phenomenon well established for quantum mechanical two-level systems. Here, we present classical two mode interference of a nanomechanical two-mode system, realizing a classical analog of Stückelberg interferometry. Our experiment relies on the coherent energy exchange between two strongly coupled, high quality factor nanomechanical resonator modes. Furthermore, we discuss an exact theoretical solution for the double passage Stückelberg problem by expanding the established finite time Landau-Zener single passage solution. For the parameter regime explored in the experiment, we find the Stückelberg return probability in the classical version of the problem to formally coincide with the quantum case which reveals the analogy of the return probabilities in the quantum mechanical and the classical version of the problem. This result qualifies classical two-mode systems at large to simulate quantum mechanical interferometry.

TT 32.2 Tue 14:15 HSZ 201

Transmon qubits meet cavity electromechanics — •P. Schmidt[1,2,3], D. Schwienbacher[1,2,3], M. Pernpeintner[1,2,3], F. Wulschner[1,2,3], F. Deppe[1,2,3], A. Marx[1,2], R. Gross[1,2,3], and H. Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Germany — [2]Physik-Department, TUM, Germany — [3]Nanosystems Initiative Munich, Germany

In cavity electromechanics, quantum mechanical phenomena can be studied in the literal sense. For the preparation of mechanical (phonon) Fock states, the integration of a sufficiently nonlinear circuit element is of key importance. Here, we present a hybrid system consisting of a superconducting coplanar microwave resonator coupled to a nanomechanical beam and a transmon qubit acting as nonlinear circuit element. In this way circuit QED is combined with the world of circuit electronanomechanics. We show continuous wave spectroscopy data for the transmon qubit as well as the nano-mechanical beam. The ac-Stark shift of the transmon qubit as well as electromechanically induced absorption measurements allow us to determine the microwave photon number in the microwave resonator for two opposite power regimes, differing by ten orders of magnitude. In both regimes we find qualitatively the same dependence of the photon number on the power applied to the microwave resonator. Our experiments demonstrate the successful combination of circuit QED and nanomechanics.

TT 32.3 Tue 14:30 HSZ 201

Frequency tuning and coherent dynamics of two nanostring resonators in the strong coupling regime — Matthias Pernpeintner[1,3], •Daniel Schwienbacher[1,2,3], Philip Schmidt[1,2,3], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Germany — [2]Physik-Department, Technische Universität München, Germany — [3]Nanosystems Initiative Munich (NIM), Germany

Coupled nanomechanical resonators are prime examples for studying synchronization effects and nonlinear dynamics. Additionally, high-quality resonators are considered as building blocks for all-mechanical information processing platforms [1,2].This, however, requires the possibility to tune the relevant mode frequencies independently and to operate the resonators in the strong coupling regime. Here, we present a possible realization consisting of two high-quality ($Q \approx 10^5$) SiN nanostring resonators in the MHz regime, coupled mechanically by a shared support. We demonstrate that the fundamental mode frequencies of both nanostrings can be tuned independently by a strong drive tone resonant with one of the higher harmonic modes. We investigate the coherent dynamics of the two strongly-coupled nanostring resonators acting as an effective classical two-level system. We discuss the observation of classical Rabi oscillations and classical Landau-Zener dynamics indicating coherent and selective phonon transfer between two spatially separated mechanical resonators.

[1] Hatanaka et al., Appl. Phys. Lett. **102**, 213102 (2013)
[2] Mahboob et al., Sci. Rep. **4**, 4448 (2014).

TT 32.4 Tue 14:45 HSZ 201

High Quality Factor Mechanical Resonator based on encapsulated $NbSe_2$ Membranes — •Markus Müller[1], Marco Will[1], Matthew Hamer[2], Roman Gorbachev[2], Adrian Bachtold[3], Christoph Stampfer[1], and Johannes Güttinger[1] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen — [2]School of Physics and Astronomy and Manchester Centre for Mesoscience and Nanotechnology, University of Manchester, Oxford Road, Manchester M13 9PL — [3]ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Barcelona

Nanomechanical resonators based on 2d materials show high mechanical quality factors and extraordinary force sensitivities. A common problem limiting graphene based resonators are electronical losses due to charge movements induced by mechanical motion or the electrical readout. One promising way to overcome this issue are superconducting 2d membranes potentially suppressing electrical losses. Here we demonstrate a hybrid membrane composed of superconducting three layer thick $NbSe_2$ encapsulated in 1-2 layers of graphene. The resonator is probed by means of capacitive coupling to a superconducting microwave cavity enabling high precision readout of the resonance frequency. We measure a mechanical quality factor of over 200,000 showing the general applicability of such heterostructures in resonators. Additionally, the quality factor is more stable in comparison to graphene only resonators when varying the gate voltage, which can be attributed to a reduced electrical resistance.

TT 32.5 Tue 15:00 HSZ 201

Hypersound spacerless cavities — •M. Esmann[1], F. Lamberti[1], O. Krebs[1], L. Lanco[1], I. Favero[2], P. Senellart[1], A. Lemaître[1], C. Gomez[1], and N.D. Lanzillotti-Kimura[1] — [1]Centre de Nanosciences et des Nanotechnologies, CNRS, Université Paris-Sud, Université Paris-Saclay, 91460 Marcoussis, France — [2]Université Paris Diderot, Sorbonne Paris Cité, Laboratoire Matériaux et Phénoménes Quantiques, CNRS-UMR 7162, 75013 Paris, France

We introduce new strategies to engineer and study semiconductor nanostructures capable of confining, controlling the propagation, and manipulating acoustic phonons in the GHz-THz frequency range. Superlattices work as high reflectance phononic mirrors and constitute a fundamental building block for the conception of more complex devices. Acoustic cavities are capable of confining and amplifying the hypersound field both spatially and in the spectral domains. Usually, an acoustic cavity is formed by two identical distributed Bragg reflectors embedding an acoustic spacer, acting in a similar way to a Fabry-Perot resonator. We design a novel kind of phononic cavities where no spacer is needed, based on the engineering of the phonon phase in the interface between two superlattices. Such kind of resonators can be combined in coupled-acoustic cavity structures such as molecules and coupled-resonator waveguides able to evidence novel physical phenomena such as acoustic Bloch oscillations.

[1] A. Fainstein et al. PRL 110, 037403 (2013)
[2] M. Xiao et al. Nature Physics 11, 240 (2015)

TT 33: Transport: Majorana Fermions

Time: Tuesday 14:00–16:00 Location: HSZ 204

TT 33.1 Tue 14:00 HSZ 204

Subband-mixing signatures in Andreev-reflection-enhanced conductance of a quantum point contact — Michal Nowak and •Michael Wimmer — QuTech and Kavli institute of nanoscience, TU Delft, Netherlands

Andreev reflection leads enhancement of the conductance in a quantum point contact, doubling the conductance plateaus [1]. Recent experiments [2, 3] found evidence for this Andreev enhancement, but showed additional, pronounced conductance dips before the transition to the next plateau, at odds with the conductance doubling of [1].

Here, we show that scattering between subbands due to weak disorder can fully explain these observations. This allows to give an estimate for the mean free path in Majorana devices [3].

[1] C.W.J. Beenakker. Phys. Rev. B 46, 12841 (1997)
[2] M. Kjaergaard *et al.*, Nat. Commun. 7, 12841 (2016)
[3] H. Zhang *et al.*, arXiv:1603.01852

TT 33.2 Tue 14:15 HSZ 204

Gapless Andreev Bound States in HgTe based topological Josephson junctions — •Jonas Wiedenmann[1], Erwann Bocquillon[1], Russel Deacon[2], Teun Klapwijk[3], Philipp Leubner[1], Christoph Brüne[1], Seigo Tarucha[2], Koji Ishibashi[2], Hartmut Buhmann[1], and Laurens Molenkamp[1] — [1]Physikalisches Institut 3, Am Hubland, Universität Würzburg — [2]Advanced Device Laboratory, Riken, Japan — [3]Kavli Institute of Nanoscience, Delf, The Netherlands

Due to their inverted bandstructure, HgTe quantum wells of appropriate thickness are a 2D TI and exhibit the Quantum Spin Hall effect. Such a topological insulator in proximity with a conventional superconductor is predicted to lead to the emergence of induced p-wave superconductivity. Majorana bound states occur as zero energy states in vortices or at edges of such a triplet pairing superconductors. In this talk I will focus on detecting two experimental signatures of such zero energy states. We show from the ac Josephson effect that the supercurrent across such a Josephson junction made of a HgTe based topological insulator, varies 4π periodically with the superconducting phase difference. Namely we identify a doubling of the Shapiro steps compared to conventional superconductors [1] and measure Josephson emission at half the Josephson frequency [2]. Furthermore, by applying a magnetic flux to the junction, we are able show that the supercurrent is predominantly carried by states edge states.

[1] Bocquillon et al. Nat. Nano (2016)
[2] Deacon et al. arXiv:1603.09611

TT 33.3 Tue 14:30 HSZ 204

The fermion parity relaxation in the topological Josephson junction — •Oleksiy Kashuba and Björn Trauzettel — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg

The topological Josephson junction is notable for its Andreev level whose energy is 4π periodic in superconducting phase. Being protected by the fermionic parity conservation, the level is supposed to provide the 4π periodic contribution to the supercurrent in addition to the conventional 2π periodicity caused by other levels. In the static experimental setup, however, even a weakest relaxation of the fermionic parity results in the pure 2π supercurrent periodicity. This problem can be in principle eliminated by the dynamically driven phase on the time scales much smaller than relaxation time. In our work we demonstrate that even in the dynamic experiments, the pseudo-equilibrium occupation of the topological level plays a crucial role, and a number of special requirements has to be met in order to obtain a non-zero 4π periodic behavior. For example: The phase should not be driven uniformly, e.g. in the voltage driven Josephson junction the current contribution from the topological Andreev level is zero; the Josephson junction driven by a constant current, i.e. resistively shunted junction (RSJ) model reveals the 4π periodicity only in the case if both 2π and 4π levels are present.

TT 33.4 Tue 14:45 HSZ 204

Josephson effect in topologically confined channels — •Daniel Frombach and Patrik Recher — Institut für Mathematische Physik, TU Braunschweig

In recent times the fractional Josephson effect has been used as a signature of Majorana fermions forming in Josephson junctions mediated by the topologically protected spin helical edge states of a quantum spin Hall insulator [1].

Here we propose a setup based on silicene in which either a single spin helical Kramers pair of edge states [2] or two sets of Kramers pair edge stets can exist at domain walls depending on an externally applied inhomogeneous electrical field. We furthermore investigate a Josephson junction mediated by these edge states through the Bogoliubov de Gennes formalism. We show that the energy phase relation is 4π periodic when the system is in the quantum spin Hall regime but changes to a 2π periodicity due to backscattering effects when two sets of Kramers pair edge states are present.

[1] L. Fu and C.L. Kane, Phys. Rev. B 79, 161408 (2009).
[2] M. Ezawa, New Journal of Physics 14, 033003 (2012).

TT 33.5 Tue 15:00 HSZ 204

Fano resonances in transport through Majorana networks — •Alexander Schuray, Luzie Weithofer, and Patrik Recher — TU Braunschweig, Institute of Mathematical Physics

Electronic transport experiments with nanowires in proximity to a superconductor [1] suggest the existence of exotic emergent particles namely Majorana bound states (MBS), which are promising candidates for topological quantum computation [2].

Transport experiments using quantum dots (QDs) coupled to MBS have been proposed [3] as the parameters of the dot may be a handle to find unique signatures of the MBS. In contrast to these previous works, we study a system in which a one dimensional topological superconductor is contacted with a normal conducting lead at one end and a QD at its other end. To obtain the transport properties of such a setup we use a Keldysh Green's function method [4]. We show that in this setup two Fano resonances which are symmetric with respect to the energy level of the QD arise. Moreover, this symmetry is only destroyed by long range tunneling terms and so is a unique signature of the topologically protected MBS. Furthermore, we verify our effective model calculations with numerical results for a Kitaev chain.

[1] V. Mourik et al., Science 336, 1003 (2012)
[2] T. Karzig et al., arXiv:1610.05289 (2016)
[3] M. Leijnse, and K. Flensberg, Phys. Rev. B 84, 1400501 (2011)
[4] L. Weithofer, P. Recher, and T. L. Schmidt, Phys. Rev. B 90, 205416 (2014)

TT 33.6 Tue 15:15 HSZ 204

Non-equilibrium Andreev States Population in Short Conventional and Topological Superconducting Junctions — •Raffael Klees, Wolfgang Belzig, and Gianluca Rastelli — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

Recent experiments reported the observation of the non-equilibrium dynamics of the Andreev bound states (ABS) in superconducting atomic contacts (SAC) [1] and in proximized semiconductor nanowires [2]. Motivated by these reports, we study a short superconducting junction of length $L \ll \xi$ (coherence length) inserted in a dc-SQUID and coupled to an LC-resonator [2]. We calculate the non-equilibrium occupation of the ABS by taking into account the phase fluctuations in the dc-SQUID and by assuming that the junction is irradiated with photons. We analyse the role of the non-equilibrium distribution of the quasiparticles of the continuum in different regimes. We systematically compare the cases of a SAC and a topological junction [3] in order to point out the peculiar features of the latter. Finally, we discuss how to measure such a non-equilibrium occupation in experiments similar to [1].

[1] C. Janvier *et al.*, Science **349**, 1199 (2015); L. Bretheau *et al.*, Nature **499**, 312 (2013)
[2] A. P. Higginbotham *et al.*, Nat. Phys. **11**, 1017 (2015)
[3] J. I. Väyrynen *et al.*, Phys. Rev. B **92**, 134508 (2015)

TT 33.7 Tue 15:30 HSZ 204

Helical gaps in interacting Rashba wires at low electron densities — •Thomas Schmidt and Christopher Pedder — Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg

Rashba spin-orbit coupling and a magnetic field perpendicular to the Rashba axis have been predicted to open a partial gap ("helical gap") in the energy spectrum of noninteracting or weakly interacting one-dimensional quantum wires. By comparing kinetic energy and Coulomb energy we show that this gap opening typically occurs at low electron densities where the Coulomb energy dominates. To address this strongly correlated limit, we investigate 1D and quasi-1D Rashba wires using Wigner crystal theory. We find that in the 1D case, the helical gap exists even in the limit of strong interactions but its dependence on electron density differs significantly from the weakly interacting case. In the quasi-1D case, we find that a helical gap can open even without applied magnetic field.

TT 33.8 Tue 15:45 HSZ 204

Evolution of the transmission phase through a Coulomb-blockaded proximitised wire — •Casper Drukier[1], Bernd Rosenow[1], and Yuval Oreg[2] — [1]University of Leipzig, Leipzig, Germany — [2]Weizmann Institute of Science, Rehovot, Israel

We present a study of the transmission of electrons through a semiconductor quantum wire with strong spin-orbit coupling in proximity to an s-wave superconductor, which is Coulomb-blockaded. Such a system supports Majorana bound states in the presence of an external magnetic field, and is of interest due to recent experimental progress and the prospect of quantum information processing.

Without superconductivity, phase lapses are expected to occur in the transmission phase. We find that they disappear when a topological superconducting phase is stabilised. We derive a model, based on an expansion in terms of Bogoliubov quasi-particles, which allows us to express tunneling through the nanowire with the help of effective matrix elements, which depend on both the fermion parity of the wire and the overlap with Bogoliubov-de-Gennes wave-functions. Using the scattering matrix formalism this allows us to study the transmission phase in different regimes.

TT 34: Spintronics, incl. Quantum Dynamics (joint session DS, HL, MA, TT, organized by MA)

Time: Tuesday 14:00–15:45 Location: HSZ 301

TT 34.1 Tue 14:00 HSZ 301

Prediction of an intrinsic spin Hall effect without spin-orbit coupling in non-collinear antiferromagnets — •Yang Zhang[1,2], Jakub Zelezny[1], Jeroen van den Brink[2], Claudia Felser[1], and Binghai Yan[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [3]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden,Germany

The spin Hall effect (SHE), which converts a charge current into a transverse spin current, has long been believed to be a phenomenon induced by the spin-orbit coupling. In this work, we have revealed the existence of an intrinsic SHE without the spin-orbit coupling by theoretical calculations. Such a SHE is realised in the chiral spin structure of non-collinear antiferromagnets, even when the scalar spin chirality is zero. We have obtained large intrinsic spin Hall conductivity in related compounds Mn 3 Ge and Mn 3 Sn, that are chiral antiferromagnetic above room temperature and also predicted to be Weyl semimetals recently. Our work provides further understanding on the spin Hall effect and paves a new way to design SHE materials based on the chiral magnetic materials.

TT 34.2 Tue 14:15 HSZ 301

Ising spintronics in transition-metal dichalcognides — •Bin Shao[1], Malte Schüler[1,2], Gunnar Schönhoff[1,2], Thomas Frauenheim[1], Gerd Czycholl[2], and Tim Wehling[1,2] — [1]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany — [2]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

The orbital character of charge carriers at the Fermi level of transition-metal dichalcognides, MX_2 (M = Mo, W; X = S, Se, Te), can be selected via doping levels, leading to orbital dependent spin-flip scatterings with magnetic adatoms on MX_2. By utilizing this feature, we propose a mechanism for Ising spintronics relying on the tunability of spin lifetime of transition-metal adatoms with d^9 configuration on a MX_2 monolayer. The spin lifetime can be tuned by more than two orders by shifting the Fermi level only slightly. Moreover, the system exhibits a sizable magnetic anisotropy. We calculate the spin lifetime and magnetic anisotropy of magnetic adatoms based on an effective model Hamiltonian, reveling their connections to doping levels and the symmetry of adsorption sites straightforwardly. Our *ab initio* calculations suggest that this Ising-type spintronics should be realizable in Co, Rh, or Ir adatoms on MoS_2.

TT 34.3 Tue 14:30 HSZ 301

A three-input majority gate with chiral magnetic solitons —

Konstantinos Koumpouras[1], Dmitry Yudin[2], Danny Thonig[1], Christoph Adelmann[3], Anders Bergman[1], Olle Eriksson[1], and •Manuel Pereiro[1] — [1]Department of Physics and Astronomy, University Uppsala, Sweden — [2]ITMO University, Saint Petersburg 197101, Russia — [3]IMEC vzw. Kapeldreef 75, B-3001 Leuven, Belgium

In magnetic materials, nontrivial spin textures may emerge owing to the competition among different types of magnetic interactions. In particular, chiral magnetic solitons, represent topologically protected spin configuration with particle-like properties, that are ideally suited to perform logical operations. Based on atomistic spin dynamics simulations, we propose to make use of magnetic solitons in a functional and dynamic three-input majority gate, in which the input states can be controlled by applying an external electromagnetic field or spin-polarized currents. One of the main advantages of the proposed device is that the input and output signals are encoded in the chirality of solitons, allowing to perform logical operations. As examples we illustrate how the proposed device can be used to perform logical relations such as Boolean AND and OR.

TT 34.4 Tue 14:45 HSZ 301

Spin-torque Effects in Thermally Assisted Magnetization Reversal: Kramers' Escape Rate Theory Approach — Yuri P. Kalmykov[1], Declan J. Byrne[2], •William T. Coffey[3], William J. Dowling[3], Sergey V. Titov[4], and Jean Eric Wegrowe[5] — [1]Univ. Perpignan Via Domitia, Laboratoire de Mathématiques et Physique, F-66860, Perpignan, France — [2]School of Physics, University College Dublin, Belfield, Dublin 4, Ireland — [3]Department of Electronic and Electrical Engineering, Trinity College, Dublin 2, Ireland — [4]Kotel'nikov Institute of Radio Engineering and Electronics of the Russian Academy of Sciences, Vvedenskii Square 1, Fryazino, Moscow Region, 141120, Russia — [5]Laboratoire des Solides Irradiés, Ecole Polytechnique, 91128 Palaiseau Cedex, France

Thermal fluctuations of nanomagnets driven by spin-polarized currents are treated via the Landau-Lifshitz-Gilbert equation generalized to include both the random thermal noise field and the Slonczewski spin-transfer torque (STT) term. The reversal time of the magnetization in such a nanomagnet are evaluated for wide ranges of damping by using the method of Coffey et al. [Phys. Rev. E 63, 021102 (2001)]. Their method generalizes the Mel'nikov-Meshkov approach [J. Chem. Phys. 85, 1018 (1986)] for bridging the very low damping (VLD) and intermediate damping (ID) Kramers escape rates for mechanical Brownian particles (the Kramers turnover problem) to the analogous magnetic turnover problem.

TT 34.5 Tue 15:00 HSZ 301

Inducing spin in semiconducting 2D phosphorene — •Mukul Kabir — Department of Physics, and Centre for Energy Science, Indian Institute of Science Education and Research, Pune, India

Inducing magnetic moment in otherwise nonmagnetic two-dimensional semiconducting materials is the key first step to design spintronic materials. In this talk, we will address the feasibility of inducing such local moment in single-layer phosphorene through 3d transition-metal (TM) doping without affecting its intrinsic semiconducting nature. While adjudicating on this subject, all previous studies conveniently neglected TM diffusion. However, we predict that increased TM diffusivity on pristine phosphorene would severely hinder any possibility of controlled magnetism, and thus any application. Here we propose that the point-defects will anchor metals, and exponentially reduce the diffusivity. We further argue that the divacancy complex is imperative in any practical purpose due to their increased thermodynamic stability over monovacancy. For most cases, the defect-transition metal complexes retain the intrinsic semiconducting properties, and also induce a local magnetic moment with large exchange-splitting and spin-flip energies, which are necessary for spintronic applications. Further, we provide a simple microscopic model to describe the local moment formation in these transition metal and defect complexes. Moreover, such metal absorption could completely alter the intrinsic electronic structure of the single-layer phosphorene, and may lead to exotic many-body physics.

TT 34.6 Tue 15:15 HSZ 301

Adsorption and element-specific detection of transition metal porphyrins by spin-dependent conductance of a graphene nanoribbon — •Peter Kratzer[1], Sherif A. Tawfik[2], Xiang Yuan Cui[2], and Catherine Stampfl[2] — [1]Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]The University of Sydney, Sydney, New South Wales 2006, Australia

Transition metal porphyrins, their adsorption on graphene nanoribbons (GNRs), and its consequences for electronic transport through the GNRs are investigated by means of density functional theory calculations. Interaction with a single-atom vacancy in the GNR is found to be a prerequisite for chemical bonding of the transition metal centre. In both the physisorbed and the chemisorbed geometry, the inclusion of van der Waals interaction results in a significant enlargement of the binding energy. Electronic transport calculations using non-equilibrium Greens functions show that the conductivity of the edge states in the GNR is altered by the chemisorbed porphyrin molecules. Since the metal centers of porphyrins carry an element-specific magnetic moment, the spin-dependence of the conductance of the GNR is altered, too. In particular, the adsorption of Ru-porphyrin or Fe-porphyrin on the single-atom vacancy results in a large spin polarization of the current of 88% and -62%, respectively, at small applied source-drain voltages. Based on our results, we suggest that a spin valve constructed from a GNR with ferromagnetic contacts could be used as a sensitive detector that could discriminate between various metal porphyrins.

TT 34.7 Tue 15:30 HSZ 301

Shape Memory Alloys in Hybrid Spintronic Devices — •Andreas Becker and Andreas Hütten — Bielefeld University, Bielefeld, Germany

Observations of the phase transition in ferromagnetic shape memory alloys (FSMAs) by x-ray diffraction and magnetization measurements are reported frequently. Our goal is to investigate the phase transformation by using the tunnel magnetoresistance effect (TMR), thus FSMAs are utilized either as ferromagnetic electrodes (Ni50-xCoxMn30Al20/MgO/ Co40Fe40B20) or as an underlying layer beneath the magnetic tunnel junction (Ni50-xCoxMn30Al20/ Co40Fe40B20/MgO/ Co40Fe40B20).

The off-stoichiometric Ni50-xCoxMn30Al20 thin films are grown by sputter deposition and patterned by e-beam lithography. X-ray diffraction measurements indicate a B2 crystal structure. An untypical change in the TMR amplitude is observed in tunnel junctions on top of the Heusler alloy upon heating the sample. We suggest that this phenomenon arises from the induced strain of the reverse martensitic transformation. Furthermore the FSMA will act as a ferromagnetic electrode if the magnetic properties are enhanced by substituting Ni with Co atoms. At x=10 a TMR of about 2.5% at room temperature and 6% at 10 K is measured in Ni50-xCoxMn30Al20 /MgO/Co40Fe40B20 tunnel junctions while no TMR is found over the measured temperature range in samples with x=4.

TT 35: Low-Dimensional Systems: 2D - Theory

Time: Tuesday 14:00–15:30 Location: HSZ 304

TT 35.1 Tue 14:00 HSZ 304

Weathervane modes of dipoles on the kagome lattice — •Mykola Maksymenko[1], Roderich Moessner[2], and Kirill Shtengel[3] — [1]Institute for Condensed Matter Physics of NAS of Ukraine, Lviv-79011, Ukraine — [2]Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany — [3]Department of Physics and Astronomy, University of California at Riverside, Riverside, CA 92521, USA

We investigate the nature of excitations in a narrow spin-wave mode of the Kagome lattice antiferromagnet in the presence of dipolar interactions. While this case is qualitatively different from the nearest-neighbour model and lacks the Heisenberg spin-rotational symmetry, even moderately strong long-range dipolar interactions preserve the narrow mode, which remains dispersionless (flat) to a good approximation.

We provide a microscopic model underpinning this phenomenon and discuss its applicability to other lattices and its stability to additional interactions.

TT 35.2 Tue 14:15 HSZ 304

Competing mass terms in Dirac fermions — •Toshihiro Sato, Martin Hohenadler, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

We numerically study the honeycomb-lattice Hubbard model at half filling coupled to a transverse Ising field. The coupling to the Ising field is such that it favors a Kekule mass term when it orders. This Kekule mass breaks translation symmetry and corresponds to a complex order parameter. The Hubbard interaction favors an antiferromagnetic state characterized by an O(3) order parameter. Using the auxiliary field quantum Monte Carlo method, we are able to map out the phase diagram in the transverse field versus Hubbard U plane so as to investigate the competition between the two aforementioned mass terms.

TT 35.3 Tue 14:30 HSZ 304

Interaction induced gap of magnetic Graphene — •zhenjiu wang and fakher. f. assaad — Institut für Theoretische Physik und Astrophysik , Universität Würzburg, Germany

We investigate the interaction induced ordered state of relativistic Landau Levels by means of unbiased lattice quantum Monte Carlo simulations. The model we consider is a Hubbard hamiltonian on the honeycomb lattice in the presence of an orbital magnetic field and supplemented by a nearest neighbor interaction such that at the classical level charge density wave and spin density wave states are degenerate. Our calculations show that the magnetic field induced flat band is unstable towards magnetic ordering. As one approaches Gross-Neveu quantum criticality the single particle gap shows a crossover behavior from linear to square root scaling as a function of magnetic field.

TT 35.4 Tue 14:45 HSZ 304

Comparison Between the Hybrid and Auxiliary Field Quantum Monte Carlo Algorithms in Condensed Matter — •Stefan Beyl, Florian Goth, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Deutschland

The Hybrid Quantum Monte Carlo (HQMC) is an established and successfully used algorithm in the lattice gauge community. A better scaling and lower memory requirements awake the hope to access larger system sizes than with the auxiliary field methods, which are generically used in condensed matter. We present results of a detailed comparisons between HQMC and auxiliary field Quantum Monte Carlo simulations on the Hubbard model. Furthermore, we show HQMC results for electron phonon simulations.

TT 35.5 Tue 15:00 HSZ 304

Spontaneous particle-hole symmetry breaking of correlated fermions on the Lieb lattice — •Martin Bercx[1], Johannes S. Hofmann[1], Fakher F. Assaad[1], and Thomas C. Lang[1,2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Institute for Theoretical Physics, University of Innsbruck, Austria

We study spinless fermions with nearest-neighbor repulsive interactions (t-V model) on the two-dimensional three-band Lieb lattice. At half-filling, the free electronic band structure consists of a flat band at zero energy and a single cone with linear dispersion. The flat band is expected to be unstable upon inclusion of electronic correlations, and a natural channel is charge order. However, due to the three-orbital unit cell, commensurate charge order implies an imbalance of electron and hole densities and therefore doping away from half-filling. Our numerical results show that below a finite-temperature Ising transition a charge density wave with one electron and two holes per unit cell and its partner under particle-hole transformation are spontaneously generated. Our calculations are based on recent advances in auxiliary-field and continuous-time quantum Monte Carlo simulations that allow sign-free simulations of spinless fermions at half-filling. It is argued that particle-hole symmetry breaking provides a route to access levels of finite doping, without introducing a sign problem.

TT 35.6 Tue 15:15 HSZ 304

Field Theoretical Aspects of Quantum Hall States — •Christian Tutschku, Jan Böttcher, and Ewelina M. Hankiewicz — Institut für Theoretische Physik und Astronomie, Uni Würzburg, 97074 Würzburg, Germany

In condensed matter physics the family of Quantum-Hall (QH) states is one of the most fascinating examples for macroscopic measurable quantum effects. Moreover, the integer, the fractional, the anomalous and the quantum spin Hall effect are of special interest due to their topological origin [1]. All these effects could be described via 2+1 dimensional gauge theories, including topological Chern-Simons (CS) tensor structures of characteristic level [2]. Even if the bare Lagrangian of a theory does not include a CS term, it could be generated at one loop level via contributions of the vacuum polarization operator [3]. If the bare Lagrangian is invariant under a certain symmetry transformation, the one loop correction may also induce an anomaly, which could be related to nonzero off-diagonal eigenvalues of the conductivity tensor [4]. We analyze the formation of CS terms in quantum field theories, describing the different QH states, and show that these terms characterize their topological invariant, their conductivity tensor and their (fractional) statistics. Moreover, we illustrate that the parity anomaly leads to an anomalous QH current.

[1] D. Tong, arXiv:1606.06687 (2016)
[2] G. V. Dunne, arXiv:hep-th/9902115 (1999)
[3] V. R. Khalilov, Theor. Math. Phys. 125 (2000)
[4] A. N. Redlich, Phys. Rev. D 29, 2366 (1984)

TT 36: Brownian Motion (jointly with DY)

Time: Tuesday 10:00–13:00 Location: ZEU 147

TT 36.1 Tue 10:00 ZEU 147

Convex Hulls of Random Walks in High Dimensions: A Large-Deviation Study — •Hendrik Schawe[1], Alexander K. Hartmann[1], and Satya N. Majumdar[2] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [2]Laboratoire de Physique Théorique et Modèles Statistiques, Université de Paris-Sud

We study the convex hulls of random walks in high dimensions, i.e., the smallest convex polytope enclosing the trajectory of a random walk with T steps. While the convex hulls of two-dimensional random walks are decently studied [1, 2], very little is known about the convex hulls of random walks in $d \geq 3$. Using Markov chain Monte Carlo sampling-techniques, we can study a large part of the support of the distributions of the volume V of the convex hulls or its surface ∂V. This enables us to reach probability densities below $P(A) = 10^{-800}$ and scrutinize large-deviation properties. Similar to two-dimensional random walks, the probability densities show a universal scaling behavior dependent on the exponent $\nu = 0.5$ and the *effective* dimension of the observable, i.e., $d_{\text{eff}} = d$ for V and $d_{\text{eff}} = d-1$ for ∂V. Further, we determined the rate function $\Phi(\cdot) = -\frac{1}{T}\log P(\cdot)$ which shows convergence to a limit shape for $T \to \infty$, which seems to be a power law with an exponent only dependent on d_{eff} and ν.

[1] G. Claussen, A. K. Hartmann, and S. N. Majumdar, Phys. Rev. E **91**, 052104 (2015); [2] T. Dewenter, G. Claussen, A. K. Hartmann, and S. N. Majumdar, Phys. Rev. E **94**, 052120 (2016)

TT 36.2 Tue 10:15 ZEU 147

The transient subdiffusive behavior of particles in mucus — •Thomas John[1], Matthias Ernst[2], Marco Günther[2], Ulrich Schäfer[3], Christian Wagner[1], and Claus-Michael Lehr[4] — [1]Experimental Physics, University of Saarland — [2]Faculty of Engineering, University of Applied Sciences, Saarbrücken — [3]Helmholtz Institute for Pharmaceutical Research Saarland — [4]Biopharmaceutics and Pharmaceutical Technology, University of Saarland

Biological barriers are crucial in protecting our body from environmental influences. Well-known outer barriers are intestinal, pulmonary, nasal, buccal, cervico-vaginal and dermal barriers. Except for the dermal barrier, all these are covered by a mucus layer, providing an additional barrier to the epithelial cell layer.

We have applied a model to explain the reported subdiffusion of particles in mucus, based on the measured mean squared displacements (MSD). The model considers Brownian diffusion of particles in a confined geometry, made from permeable membranes. The applied model predicts a normal diffusive behavior at very short and long time lags, as observed in several experiments. In between these time scales, we find that the "subdiffusive" regime is only a transient effect, $MSD \propto \tau^{\alpha}$, $\alpha < 1$. The only parameters in the model are the diffusion-coefficients at the limits of very short and long times, and the distance between the permeable membranes L. Our numerical results are in agreement with published experimental data for realistic assumptions of these parameters.

This work was submitted and accepted in the Biophysical Journal.

TT 36.3 Tue 10:30 ZEU 147

Non-Gaussian Statistics of Tracer Positions in Fluids Stirred by Microswimmers — •Thomas John[1], Levke Ortlieb[1], Philippe Peyla[2], Salima Rafaï[2], and Christian Wagner[1] — [1]Experimental physics University of Saarland — [2]Laboratoire Interdisciplinaire de Physique, Grenoble

We performed statistical analyses on the measured positions of μm-sized tracer particles in liquids stirred by the microswimmer *Chlamydomonas reinhardtii*. Various tracer diameters, swimmer concentrations and mean swimmer velocities were examined. The statistical characteristics are compared with predictions from various models. Our observed mean squared displacement of the tracer is linear over more than two order of magnitudes in time. The underlying probability density function ($pdf(\Delta t)$) of the displacements has a Gaussian core from the Brownian motion and non-Gaussian tails from the interactions with the flow field from the swimmers. The *pdf* shows a transient diffusive scaling behavior at short times. This scaling breaks down at times longer than few seconds. Our results are in very good agreement with the predictions of the microscopic model by Thiffeault, PRE **92** 023023(2015).

TT 36.4 Tue 10:45 ZEU 147

Dynamically Crowded Solutions of Brownian Needles — •Sebastian Leitmann[1], Felix Höfling[2], and Thomas Franosch[1] — [1]Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21A, A-6020 Innsbruck, Austria — [2]Fachbereich Mathematik und Informatik, Freie Universität Berlin, Arnimallee 6, 14195 Berlin, Germany

We perform Brownian dynamics simulations of solutions of infinitely thin needles up to densities n deep in the semidilute regime. With increasing density, the motion of a needle becomes increasingly restricted to a sliding back-and-forth movement in a tube composed of the surrounding needles. From the density-dependent behavior of the rotation and the translation we extract the corresponding longtime transport coefficients and corroborate the scaling behavior of $\sim n^{-2}$. The characteristic algebraic decay of $\sim t^{-1/2}$ in the intermediate scattering function and a plateau over many decades in time in the non-Gaussian parameter represent a fingerprint of the sliding motion of the needle within the tube. We show that on coarse-grained time and length scales, the dynamics of a needle in solution is captured by a single needle (phantom needle) with the extracted transport coefficients as input parameters [1] as anticipated from the tube theory of Doi and Edwards [2]. We also compare the dynamics to needle Lorentz systems where a single tracer needle explores a quenched array of other needles.

[1] S. Leitmann, F. Höfling, and T. Franosch, Phys. Rev. Lett. 117, 097801 (2016). [2] M. Doi and S. F. Edwards, J. Chem. Soc., Faraday Trans. 2 74, 560 (1978).

TT 36.5 Tue 11:00 ZEU 147

Electronic and photonic counting statistics as probes of non-equilibrium quantum dynamics — •Björn Kubala[1], Joachim Ankerhold[1], and Andrew D. Armour[2] — [1]Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany — [2]School of Physics and Astronomy, University of Nottingham, Nottingham, UK

The emission of radiation generated by the flow of charges through a mesoscopic conductor depends not just on the properties of the conductor itself, but also on those of its electromagnetic environment. Coupling a conductor to a high-quality electromagnetic cavity generates strong mutual feedback which can lead to novel far-from-equilibrium regimes where the charge current and the photon flux leaking out of the cavity are both determined by the nonlinear behavior of the combined system. Using a voltage-biased Josephson junction as an example, we investigate how the photonic and charge current statistics are related to each other and to the underlying coupled dynamics in the non-equilibrium regime. We demonstrate that there is a simple connection between the full counting statistics of the charges and the photons in the long time limit. We also show that measurements of photon statistics would signal the crossover from linear to nonlinear dynamics in the conductor-cavity hybrid through the emergence of highly coherent charge transport.

[1] B. Kubala, J. Ankerhold, and A. D. Armour, arXiv:1606.02200

15 min. break

TT 36.6 Tue 11:30 ZEU 147

Anomalous statistics and ergodicity breaking in a semi-classical electron transfer dynamics — •Igor Goychuk — Institute for Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam-Golm, Germany

Can statistical properties of single-electron transfer events be correctly predicted within a common equilibrium ensemble description? This fundamental in nanoworld question of ergodic behavior is scrutinized within a very basic semi-classical model of electron transfer. It is shown that in the limit of non-adiabatic electron transfer (weak tunneling) well-described by the Marcus-Levich-Dogonadze (MLD) rate the answer is yes. However, in the limit of the so-called solvent-controlled adiabatic electron transfer, a profound breaking of ergodicity occurs. Namely, for sufficiently large activation barriers, the ensemble survival probability in a state remains always nearly exponential with the inverse rate given by the sum of the adiabatic curve crossing (Kramers) time and the inverse MLD rate. In contrast, near to adiabatic regime, the single-electron survival probability is clearly non-exponential, even

though it possesses an exponential tail which agrees well with the ensemble description. Initially, it is well described by a Mittag-Leffler distribution with a fractional rate. Paradoxically, the mean transfer time in this classical on the ensemble level regime is well described by the inverse of nonadiabatic quantum tunneling rate on a single particle level. An analytical theory is developed which perfectly agrees with stochastic simulations and explains our findings.

TT 36.7 Tue 11:45 ZEU 147

Strong coupling, non-Markovian transport: Transient deviations from fluctuation-dissipation theorems — •Javier Cerrillo, Maximilian Buser, and Tobias Brandes — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

Transient dynamics of transport settings in the strong coupling and non-Markovian regimes are expected to exhibit deviations from steady state fluctuation-dissipation theorems. We show that these may be exactly quantified in terms of equilibration dynamics under alternative measurement schemes. This relation holds far from equilibrium and extends to high-order transport cumulants. In order to explore the strong-coupling, non-Markovian regime where these deviations are expected to be strongest, a new simulation method based in a hierarchy of equations of motion has been developed for the computation of arbitrary cumulants in transport settings. We instantiate our proposal with the study of deviations of high-order cumulants of energetic transport between two baths connected via a few level system.

TT 36.8 Tue 12:00 ZEU 147

Full counting statistics in the non-Markovian, strong-coupling regime - a hierarchy of equations of motion approach — •Maximilian Buser, Javier Cerrillo, and Tobias Brandes — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Within the framework of open quantum systems, we present a new numerical approach to full-counting statistics (FCS) of environmental observables. It is based on the hierarchy of equations of motion (HEOM) technique, a well-established method for the simulation of general multilevel open systems. Thereby, our method directly inherits the key advantages from the HEOM. It faithfully represents non-Markovian effects of the environment and is non-perturbative in the open system-environment coupling strength. Additionally, arbitrary time dependencies of the system Hamiltonian are correctly treated. Here, we focus on usual two-point measurement statistics and show how the back-effect accompanying the initial measurement becomes especially relevant within the now accessible regime. We exemplify our method with a discussion of energetic fluxes trough open systems which are subject to environmental far from equilibrium constraints and study the effect of time-dependent control on the system.

TT 36.9 Tue 12:15 ZEU 147

Ratchet with tunable asymmetry based on φ Josephson junction: operation, loading & efficiency. — •Edward Goldobin[1], Rosina Menditto[1], Martin Weides[2], Hermann Kohlstedt[3], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Physikalische Institut, Universität Tübingen, Auf der Morgenstelle 14, 72076, Tübingen, Germany — [2]Physikalisches Institut, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany — [3]Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel, D-24143 Kiel, Germany

We demonstrate experimentally the operation of a deterministic Josephson ratchet with tunable asymmetry [1]. The ratchet is based on a φ Josephson junction with a ferromagnetic barrier [2] operating in the underdamped regime. The ratchet operation with a load, i.e. in the presence of the additional dc counter current trying to stop the ratchet, is also demonstrated. Under these conditions the ratchet produces a non-zero output power. We estimate the efficiency of the ratchet using a general model for Josephson ratchets with hysteresis [3].

[1] R. Menditto, et al. Phys. Rev. E **94**, 042202 (2016).
[2] H. Sickinger, et al. Phys. Rev. Lett. **109**, 107002 (2012).
[3] E. Goldobin, et al., Phys. Rev. E **94**, 032203 (2016).

TT 36.10 Tue 12:30 ZEU 147

Particle transport using rocking Brownian motors — •Christian Schwemmer[1], Stefan Fringes[1,2], Colin Rawlings[1], and Armin Knoll[1] — [1]IBM Research - Zurich, Switzerland — [2]Institute of Physical Chemistry, University of Zurich, Switzerland

Inspired by how intracellular transport is achieved in nature [1], artificial Brownian motors have been designed to allow for particle transport in fluids [2]. The two main requirements are a spatially asymmetric potential and an external driving force. For our implementation, we utilize a novel approach to transport 60 nm gold particles inside a nanofluidic slit. In detail, we use the electrostatic interaction between the gold particles and surfaces to define, similar to geometry induced trapping [4], a potential landscape. Therefore, one of the confining surfaces is patterned with a 3D ratchet topography by thermal scanning probe lithography [3] which then directly translates to a potential landscape. In contrast to most previous experiments which used flashing ratchets, we realized a rocking ratchet by applying a zero-mean AC electric field across the slit delivering high particle drift speeds of up to 100 μm/s. Experimentally, we could further show that the potential landscape and thus the transport properties strongly depend on the particle size and the gap distance of the slit. By exploiting this property, we plan to develop a fast and highly selective nanoparticle sorting device.

[1] Vale et al., Science, **288**, 88, (2000)
[2] Hänggi et al., Rev. Mod. Phys, **81**, 387, (2009)
[3] Pires et al., Science, **328**, 732, (2010)
[4] Krishnan et al., Nature, **467**, 692, (2010)

TT 36.11 Tue 12:45 ZEU 147

Brownian Carnot Engine — •Edgar Roldan[1], Ignacio A. Martinez[2,3], Luis Dinis[3], Juan MR Parrondo[3], Raul A. Rica[4,5], and Dmitry Petrov[4] — [1]Max Planck Institut fur Physik Komplexer Systeme — [2]Ecole Normale Superieure de Lyon — [3]Universidad Complutense de Madrid and GISC — [4]ICFO The Institute of Photonic Sciences — [5]Universidad de Granada

The Carnot cycle imposes a fundamental upper limit to the efficiency of a macroscopic motor operating between two thermal baths. However, this bound needs to be reinterpreted at microscopic scales, where molecular motors and some artificial micro-engines, operate. Energy transfers in microscopic systems are random and thermal fluctuations induce transient decreases of entropy, allowing for possible violations of the Carnot limit. Nearly two centuries after Carnot's work, we report an experimental realization of a Carnot engine with a single optically trapped Brownian particle as the working substance. We present an exhaustive study of the energetics of the engine and analyse the fluctuations of the finite-time efficiency, showing that the Carnot bound can be surpassed for a small number of non-equilibrium cycles. As its macroscopic counterpart, the energetics of our Carnot machine exhibits basic properties that one would expect to observe in any microscopic energy transducer operating with baths at different temperatures. Our results characterize the sources of irreversibility in the engine and the statistical properties of the efficiency, an insight that could inspire new strategies in the design of efficient nano-motors.

TT 37: Graphene Posters (joint session DS, DY, HL, MA, O, TT, organized by O)

Time: Tuesday 18:30–20:30 Location: P2-EG

TT 37.1 Tue 18:30 P2-EG

Inelastic electron tunnelling into graphene bilayers on Ir(111) — •Alexander Tries, Johannes Halle, Nicolas Néel, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

Physical vapour deposition of C onto graphene-covered Ir(111) has been used to fabricate graphene nanoflakes. Due to C atom intercalation the flakes form underneath graphene. Scanning tunnelling microscopy with atomic resolution reveals that the lattices of the upper graphene layer and the flakes are rotated with respect to each other. Spectra of the differential conductance show the hole-like Ir(111) surface resonance on top of the graphene-flake stackings. Graphene phonons with wave vectors comparable to the Brillouin zone dimensions leave their signatures in inelastic electron tunnelling spectra. Funding by the Deutsche Forschungsgemeinschaft through Grant No. KR 2912/10-1 is acknowledged.

TT 37.2 Tue 18:30 P2-EG

The effect of defects on the band structure of graphene near the Dirac point — •Piotr Kot[1,2], Jonathan Parnell[2], Sina Habibian[2], and Christian R. Ast[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of British Columbia, Vancouver, Canada

Using a simple real-space tight-binding model, we present the effect of defects on the band structure of graphene in momentum space near the Dirac point. While several of the calculated defects strongly alter the band dispersion and line width near the Dirac point, we find that a band gap forms only in systems where atoms are missing from one sublattice. Another finding of note is that some specific defects open a band gap with broadened, but not entirely delocalized, states in the gap. These band gaps with broadened states strongly resemble "elongated" Dirac points that have been experimentally found by photoemission spectroscopy and have been discussed in the literature. We surmise that these "elongated" Dirac points are, at least in part, due to specific defects in the graphene. Our findings also point to obstacles to opening a band gap in graphene, which have to be considered.

TT 37.3 Tue 18:30 P2-EG

Scanning tunneling microscopy and spectroscopy on graphene/*h*-BN/SiO_2/Si devices — •Lena Stoppel, Fabian Paschke, Julia Tesch, Samuel Bouvron, Yuriy S. Dedkov, and Mikhail Fonin — Department of Physics, University of Konstanz, Germany

Exceptional transport properties of graphene, a two-dimensional honeycomb lattice of sp^2-bonded carbon atoms, make it a promising material for applications in microelectronics and sensing.

Here, we present a systematic scanning tunneling microscopy (STM) study of graphene on *h*-BN/SiO_2/Si substrates. We use wet chemical transfer of CVD-grown multilayer hexagonal boron nitride (*h*-BN) and CVD-grown monolayer graphene onto a silicon chip with a thin insulating silicon dioxide layer. The transfer method was optimized in a way that STM measurements reveal large surface areas of clean graphene, showing the honeycomb atomic lattice and a Moiré pattern due to the underlying *h*-BN. We also perform scanning tunneling spectroscopy measurements to investigate the electronic properties of graphene. In a similar procedure graphene was transferred onto metal dichalcogenides, and the electronic properties were investigated.

TT 37.4 Tue 18:30 P2-EG

Novel preparation technique for high quality graphene on boron nitride samples for combined electrical transport and STM measurements — •Tjorven Johnsen, Michael Weimer, Peter Nemes-Incze, and Markus Morgenstern — II. Physikalisches Institut B, RWTH Aachen, Otto-Blumenthal-Straße, 52074 Aachen

Whereas in electrical transport experiments suspended graphene samples or samples sandwiched between to boron nitride flakes show the highest mobility due to low charge disorder they are not accessible for scanning tunneling microscopy (STM). STM requires a graphene flake that is supported by a substrate and features an exposed surface. Here we present a novel technique to prepare such graphene samples on boron nitride substrates. A mica support is used to pick up boron nitride and graphene flakes from SiO_2 substrates. The graphene flake is contacted by gold evaporation through a shadow mask. In contrast to other fabrication methods we avoid any polymers in the process that works without any wet chemistry leading to a dry and polymer free transfer and contacting process for 2D materials. In addition to the low density of adsorbates on the graphene surface the clean and flat boron nitride substrate leads to high quality graphene samples.

TT 37.5 Tue 18:30 P2-EG

Graphene growth on SiC(0001) without step bunching — •Jakob Lidzba, Martina Wanke, Florian Speck, and Thomas Seyller — Professur für Technische Physik, Institut für Physik, TU Chemnitz, Reichenhainer Straße 70, 09126 Chemnitz, Germany

Epitaxial growth of graphene on SiC(0001) is a well-established method for the production of high-quality graphene layers [1]. The growth process ist accompanied by a step bunching of the SiC and the concomitant formation of so-called macrosteps. Since the growth of graphene layers starts at the step edges, this prevents the formation of uniform graphene films. Therefore it is crucial to find a way of controlling their development. Kruskopf et al. stated, that the H-etch pretreatment is responsible for strong step bunching. However, the formation of high steps at the surface can be suppressed by separating the processes of buffer layer and graphene growth [2,3]. In this study we test different parameters for the growth process of monolayer graphene to avoid step bunching and therefore improve the growth process. Thickness of the graphene layers and chemical composition of the surface were determined from XPS spectra, while AFM was used to examine the topography of the sample surfaces.

[1] K.V. Emtsev et al., Nature Mater. **8**, 203 (2009).
[2] M. Kruskopf et al., J. Phys.: Condens. Matter **27**, 185303 (2015).
[3] M. Kruskopf et al., 2D Mater. **3**, 041002 (2016).

TT 37.6 Tue 18:30 P2-EG

Preparation of epitaxial graphene on 4H-SiC(0001) — •Hassan Kakag, Florian Speck, Martina Wanke, and Thomas Seyller — Professur für Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany

The growth of epitaxial graphene (EG) on 6H-SiC(0001) in argon under atmospheric pressure provides high-quality graphene layers at large scale [1]. The present study is focused on the optimization of hydrogen etching and growth of EG on the (0001) surfaces of the other commonly available polytype 4H-SiC. Etching in hydrogen as well as sublimation growth is carried out in a hot-wall reactor [2]. The dependence of the etching behavior on the hydrogen flow rate and annealing temperature was studied in the range of 0.2-3.0 slm and 1350-1500 °C, respectively. Furthermore, the influence of process temperature and annealing time on the graphene growth was investigated. Surface composition and graphene thickness were obtained from XPS. The surface morphology after hydrogen etching and graphene growth was investigated by AFM. The onset of graphitization is witnessed by the formation of the $(6\sqrt{3}\times6\sqrt{3})R30°$ reconstruction at 1450 °C for an annealing time of 15 min. The best result of monolayer graphene growth was achieved with an annealing time of 15 min at a temperature of 1700 °C. In addition, bilayer graphene growth at step edges of the terraced SiC substrate was observed at 15 and 30 min annealing time. The substrate steps are mostly ordered and of similar height.

[1] K. V. Emtsev et al., Nature Mater. **8**, 203 (2009).
[2] M. Ostler et al., Phys. Status Solidi B **247**, 2924 (2010).

TT 37.7 Tue 18:30 P2-EG

Role of the tunnelling junction elements in photon emission from Au/Mica, Au/Cr/Mica, graphene/Cu systems — •Hakki Tunç Çiftçi[1], Berk Zengin[1], Umut Kamber[1], Cem Kincal[1], Dilek Yildiz[1,2], and Oğuzhan Gürlü[1] — [1]Istanbul Technical University, Istanbul, Turkey — [2]University of Basel, Basel, Switzerland

Photon emission occurrence from the tunnel junction relies on the material, apex and the cleanness of the tip of a scanning tunnelling microscope (STM). Certainly the surface electronic properties of the sample as well as its morphology directly determines the nature of the emitted photons. Minute and almost untraceable variance of chemical composition of the surfaces has a serious effect on the same phe-

nomenon. For instance, chromium diffusion on to the surface in the Au/Cr/Mica system was shown to affect the local photon emission properties of the Au surface due to tunnelling injected electrons. The knowhow gathered from such studies was employed in the investigation of the photon emission measurements performed with a photon STM on Graphene/Copper system. Being able to identify the influence of tip effects and the local chemistry of the surface paved the way to a deconvoluted method of investigation of the correlation between photon emissivity of Graphene/Cu interface to the local surface orientation.

TT 37.8 Tue 18:30 P2-EG

Graphene formation on thin epitaxial grown Cu(111)-foils by chemical vapor deposition of acetone — •Jens Neurohr[1], Samuel Grandthyll[1], Michael Weinl[2], Matthias Schreck[2], Karin Jacobs[1], and Frank Müller[1] — [1]Experimental Physics, Saarland University, 66041 Saarbruecken, Germany — [2]Experimental Physics 4, University of Augsburg, 86135 Augsburg, Germany

In comparison to the standard growth of graphene on copper via the CVD-process, an oxygen containing precursor (acetone) has been used for graphene formation on thin single crystalline Cu(111-foils. In contrast to some literature reports, graphene formation can be obtained at quite low temperatures of about 700°C [1,2]. Graphene growth on the Cu(111)-foils was investigated by X-ray photoelectron spectroscopy (XPS), X-ray photoelectron diffraction (XPD), low energy electron diffraction (LEED), Fermi surface mapping(FSM), and scanning tunnel microscopy (STM) revealing nearly one monolayer coverage of mostly ±1.65° rotated domains.

References:
[1] L. Gao, J. R. Guestand N. P. Guisinger Nano Letters 10.1021/nl1016706
[2] H. K. Yu, K. Balasubramanian, K. Kim, J.-L. Lee, M. Maiti, C. Ropers, J. Krieg, K. Kern and A. M. Wodtke ACS Nano 10.1021/nn503476

TT 37.9 Tue 18:30 P2-EG

Analysis of local variations of the electronic properties of monolayer and bilayer graphene/HOPG — •Anne Holtsch and Uwe Hartmann — Universität des Saarlandes, P.O. Box 151150, 66041 Saarbrücken

Cleaving a hopg bulk material can occasionally result in formation of graphene. Compared to other substrates hopg has the advantage that occurring Moiré patterns solely have their origin in rotation of the graphene lattice with respect to the hopg lattice orientation. We investigate the topography of the Moiré superstructure by scanning tunnelling measurement (STM) and changes of the electronic properties of graphene induced by the Moiré pattern and variation in amount of graphene layers using scanning tunnelling spectroscopy (STS).

The formation of a Moiré pattern goes along with corrugation of the graphene sheet. But STM measurements of bilayer graphene where both layers are aligned without rotation but the system itself is rotated towards the substrate do not show any corrugation. A possible Moiré pattern in the lower layer does not permeate to the top layer leading to the conclusion that the occurrence of a Moiré pattern is an effect restricted to the topmost graphene layer.

In a monolayer graphene with corrugation due to a Moiré pattern the distance of the graphene layer to the substrate adjusts the size of a band gap opening. For small distance the monolayer can behave bilayer-like. With increasing distance the size of the band gap decreases.

TT 37.10 Tue 18:30 P2-EG

Sulfur intercalation of epitaxial graphene on 6H-SiC(0001) — •Santha J. Panigrahi, Florian Speck, Adrian Schütze, Martina Wanke, and Thomas Seyller — Professur für Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany

During the initial stages of the sublimation growth of epitaxial graphene on SiC(0001), a carbon-rich $(6\sqrt{3} \times 6\sqrt{3})R30°$ reconstruction, also referred to as buffer layer (BL), is formed at the interface to the SiC. Despite being structurally graphene-like, covalent interaction with the topmost Si atoms of the substrate renders the BL electronically inactive. Upon intercalation, these bonds to the substrate are broken. The BL is decoupled from the SiC substrate and the electronic properties of graphene are restored.

In this contribution, we show that upon annealing in a CVD-like setup at temperatures between 600 and 850 °C in the presence of sulfur, the BL can be decoupled from the SiC substrate. We investigate the sulfur intercalation employing a combination of experimental techniques such as X-ray photoelectron spectroscopy, low energy electron diffraction and atomic force microscopy to study chemical composition and structural properties.

TT 37.11 Tue 18:30 P2-EG

Dimerization of activated Coronene on HOPG — •Jürgen Weippert[1], Julian Bachmann[1], Jean-Francois Greisch[1,2], Artur Böttcher[1], and Manfred M. Kappes[1,2] — [1]Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

We have studied the dimerization of Coronene (Cor) as a model reaction for the fabrication of tailored graphene nanoribbons (GNR). Low energy ion beam deposition of both intact monomers as well as dehydrogenated congeners was used to grow the corresponding films. The composition of the incident cationic beam can be tuned by changing the electron impact energy and by varying the selected mass range. Thermal desorption measurements indicate that this leads to the on-surface formation of Cor dimers presumably already during the film growth. We find two different reaction channels: (a) 2(Cor-2H)*(Cor-2H)2 and (b) (Cor-2H)+Cor*(Cor-H)2. While the monomers sublime at 460K the dimers (Cor-2H)2 sublime around 800K. The thermal desorption spectra indicate that the binding energy and the pre-exponential factor (EB=2.9 eV, v=1017 s-1) of on-surface-formed dimers (Cor-2H)2 are comparable to that of directly deposited Dicoronylene. We have also explored the structures of the corresponding (Cor-2H)2 and (Cor-H)2 species using a combination of laser ablation and ion mobility measurements.

TT 37.12 Tue 18:30 P2-EG

Response of the electronic structure of graphene to pressure, temperature and humidity — •Haydar Altuğ Yildirim, Umut Kamber, Cem Kincal, and Oğuzhan Gürlü — Istanbul Technical University, Istanbul, Turkey

Since its first isolation, the detection of gas molecules as well as humidity and temperature by use of graphene have been a matter of interest. We have used atmospheric pressure Chemical Vapor Deposition (AP-CVD) grown graphene and various transfer techniques to produce graphene based sensors on dielectric substrates. A controlled atmosphere chamber was designed and built to investigate the response of the resistivity of graphene to varying pressure, temperature and humidity. Comparison of the measurements taken by custom made graphene devices and a precise commercial sensor have shown similar responses. Upon changing the surface temperature of the graphene device we were able to control the adsorption of the water molecules. Effects of graphene growth parameters and transfer processes on to dielectrics, as well as ageing and temperature over humidity sensing capacity of graphene based devices will be presented.

TT 37.13 Tue 18:30 P2-EG

A comparative study of the oxidation of PAHs using atomic oxygen — •Jürgen Weippert[1], Vincent Gewiese[1], Philipp Huber[1], Artur Böttcher[1], and Manfred M. Kappes[1,2] — [1]Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

We have studied the oxidation of PAH films (Coronene, Hexabenzocoronene, Rubrene) as model systems for fabrication of tailored nanographene oxides. The corresponding PAH films were grown by low energy ion beam deposition. The as-prepared PAH films were then exposed to a flux of atomic oxygen at room temperature. UPS and XPS based analysis of the chemical composition of the resulting oxidized films reveals a broad spectrum of PAH oxides dominated by epoxy and ether species. The interaction of flat PAHs with the substrate modifies the oxidation pathways in submonolayers cf. multilayers: epoxides are replaced by lactones as the dominating oxide with the exception of non-planar Rubrene. According to theoretical predictions we attribute this specific influence of theHOPG substrate to mobile epoxy functionalities which are produced by reaction of HOPG with incident O atoms. These can approach the adsorbed PAH molecules along the surface * thus destabilizing their molecular rims.

TT 37.14 Tue 18:30 P2-EG

Intercalated porphines at the BN/Cu(111) interface: structure, electronic properties and function — •Jacob Ducke[1], Alexander Riss[1], Alejandro Pérez Paz[2], Angel Rubio[3], Johannes V. Barth[1], and Willi Auwärter[1] — [1]Physik-Department E20, Technische Universität München, 85748 Garching, Germany — [2]ETSF, Universidad del País Vasco, 20018 San Sebastián, Spain — [3]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

The technological applicability of surface-supported molecular materials is often restricted by their limited stability. While covalent bonding can potentially enhance thermal stability, many of the currently researched molecular functionalities are sensitive to and impaired by the gaseous or liquid environment.

In this work we present the fabrication of heterostructures consisting of porphines that are sandwiched between a copper surface and an insulating BN monolayer. Due to the electronic transparency of the BN layer, the intercalated molecules can be characterized and manipulated using scanning tunneling microscopy (STM). While the presence of the capping BN layer influences the self-assembly, we show that intrinsic molecular functionalities as switching between different tautomers or self-metalation are preserved. Such metal/molecule/insulator structures provide an opportunity to protect organic materials from atmospheric pressure, and might also be used to control chemical reactions through geometric confinement.

TT 38: Transport: Quantum Coherence and Quantum Information Systems - Experiment (jointly with MA, HL)

Time: Wednesday 9:30–13:00 Location: HSZ 03

TT 38.1 Wed 9:30 HSZ 03

Adiabatic two-qubit state preparation in a superconducting qubit system — •Marc Ganzhorn[1], Daniel Egger[1], Andreas Fuhrer[1], Nikolaj Moll[1], Peter Mueller[1], Marco Roth[2], Sebastian Schmidt[3], and Stefan Filipp[1] — [1]IBM Schweiz, Rueschlikon, Schweiz — [2]Department fuer Physik, RWTH Aachen, Deutschland — [3]Institut fuer Theoretische Physik, ETH Zuerich, Schweiz

The adiabatic transport of a quantum system from an initial eigenstate to its final state while remaining in the instantaneous eigenstate of the driving Hamiltonian can be used for robust state preparation. With control over both qubit frequencies and qubit-qubit couplings this method can be used to drive the system from initially trivial eigenstates of the uncoupled qubits to complex entangled multi-qubit states. In the context of quantum simulation, the final state may encode a non-trivial ground-states of a complex molecule, or the solution to an optimization problem in the context of adiabatic quantum computing. Here we present experimental results on a system comprising fixed-frequency superconducting transmon qubits and a tunable coupler to adjust the qubit-qubit coupling via parametric frequency modulation. We realize different types of interaction terms by adjusting the frequency of the modulation. A slow variation of drive amplitude and phase leads to an adiabatic steering of the system to its final state showing entanglement between the qubits.

TT 38.2 Wed 9:45 HSZ 03

Second-order decoherence mechanisms of a transmon qubit probed with thermal microwave states — •Frank Deppe[1,2,3], Jan Goetz[1], Peter Eder[1,2,3], Michael Fischer[1,2,3], Stefan Pogorzalek[1,2,3], Edwar Xie[1,2,3], Kirill G. Fedorov[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), 80799 München, Germany

Using thermal microwaves as a probe, we identify three second-order decoherence mechanisms of a superconducting transmon qubit. First, we quantify the efficiency of a resonator filter in the dispersive Jaynes-Cummings regime and find evidence for parasitic loss channels. Second, we probe second-order noise in the low-frequency regime and demonstrate the expected T^3 temperature dependence of the qubit dephasing rate. Finally, we show that qubit parameter fluctuations due to two-level states are enhanced under the influence of thermal microwave states. In particular, we present experimental evidence for a model based on noninteracting two-level states.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria, and the IMPRS 'Quantum Science and Technology'.

TT 38.3 Wed 10:00 HSZ 03

Probing broadband engineered and residual environments with a transmon qubit — •P. Eder[1,2,3], F. Deppe[1,2,3], T. Le Anh[1,2], J. Goetz[1,2], M. Fischer[1,2,3], E. Xie[1,2,3], A. Marx[1], 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

Microwave beam splitters and transmon qubits are important components in circuit quantum electrodynamics (QED). Arranging two beam splitters in the form of an interferometer, we engineer a nontrivial broadband on-chip environment. We place the transmon qubit as a sensitive probe inside this environment and perform resonance fluorescence measurements. When comparing the experimental results with predictions from the spin-boson model, we find good agreement. Small deviations between experiment and theory indicate the presence of spurious electromagnetic modes. In general, our results demonstrate how to design and scale up complex circuits for experiments on propagating quantum microwaves.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria and the IMPRS 'Quantum Science and Technology'.

TT 38.4 Wed 10:15 HSZ 03

Chains of nonlinear and tunable superconducting resonators — •M. Fischer[1,2,3], P. Eder[1,2,3], J. Goetz[1,2], S. Pogorzalek[1,2], E. Xie[1,2,3], K. Fedorov[1,2], F. Deppe[1,2,3], A. Marx[1], 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

We present the theoretical analysis and experimental study of a quantum simulation system of the Bose-Hubbard Hamiltonian in the driven dissipative regime in the realm of circuit QED. The system consists of series-connected, capacitively coupled superconducting resonators which are both nonlinear and tunable. The nonlinearity is achieved by galvanically coupled SQUIDs. They are placed in the current antinode of each resonator and can be tuned by external coils and on-chip antennas.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria and the IMPRS 'Quantum Science and Technology'.

TT 38.5 Wed 10:30 HSZ 03

Towards a scalable 3D quantum memory — •Edwar Xie[1,2,3], Frank Deppe[1,2,3], Daniel Repp[2], Peter Eder[1,2,3], Michael Fischer[1,2,3], Jan Goetz[1,2,3], Kirill G. Fedorov[1], 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

For superconducting qubits dispersively coupled to 3D cavity resonators both T_1-and T_2-times in excess of 100 μs have been achieved. However, the 3D cavities are bulky in comparison with their (slightly less coherent) 2D counterparts. A more scalable device can be built by exploiting the multi-mode structure of the 3D cavity. Here, we present an experimental study on such a device: a transmon qubit capacitively coupled to two distinct modes of a single 3D cavity. We engineer the fundamental and the first harmonic mode of a single cavity in such a way, that the former one couples well to the external feedline, whereas the latter does not. The qubit is dispersively coupled to both modes with a rate $g/2\pi \simeq 60$ MHz. Using a second-order coupling protocol, we observe an enhancement in qubit lifetime by a factor of 3 compared to the pure qubit lifetime and find that this value is not limited by fundamental constraints.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria and the IMPRS 'Quantum Science and Technology'.

TT 38.6 Wed 10:45 HSZ 03

Finite-time correlations of balanced two-mode squeezed microwave states — •Kirill Fedorov[1,2], Stefan Pogorzalek[1,2], Patrick Yard[1,2], Peter Eder[1,2,3], Michael Fischer[1,2,3], Jan Goetz[1,2], Edwar Xie[1,2,3], Achim Marx[1], 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

Generation of balanced two-mode squeezed states is a key task in quantum communication and illumination with continuous variables, as it enables distribution of quantum entanglement between distant parties. For this reason, the investigation of such states is of high interest in the field of propagating quantum microwaves. In our work, we perform tomography of balanced two-mode squeezed microwave states which are created by the means of two flux-driven Josephson parametric amplifiers generating orthogonally squeezed states at the inputs of a 50 : 50 microwave beam splitter. We study finite-time correlations in order to measure a characteristic time of entanglement decay in quantum channels. Our studies show that quantum communication and illumination protocols with continuous-variable propagating microwaves are experimentally feasible.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria, and the IMPRS 'Quantum Science and Technology'.

TT 38.7 Wed 11:00 HSZ 03

Impact of noise on entanglement of two-mode squeezed microwave states — •S. Pogorzalek[1,2], K. G. Fedorov[1,2], P. Yard[1,2], P. Eder[1,2,3], M. Fischer[1,2,3], J. Goetz[1,2], E. Xie[1,2,3], A. Marx[1], F. Deppe[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

Propagating quantum signals in the form of microwave two-mode squeezed states (TMSSs) can be generated by utilizing Josephson parametric amplifiers (JPAs). In our experiments, we employ two flux-driven JPAs at the inputs of an entangling hybrid ring in order to generate TMSSs between the hybrid ring outputs. This allows us to generate quantum entangled propagating microwave signals suitable for quantum communication and sensing applications such as quantum teleportation and quantum radar. However, the performance of these schemes may drastically depend on the amount of environmental noise in the communication channels. We study this dependence experimentally by controlling the amount of excess noise in different parts of the setup. Finally, we investigate the robustness of entanglement to thermal and shot noise via a negativity criterion and determine fundamental negativity-versus-noise limits.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria, and the IMPRS 'Quantum Science and Technology'.

15 min. break.

TT 38.8 Wed 11:30 HSZ 03

Tailoring coupling in artificial superconducting quasi-spins — •Alexander Stehli, Jochen Braumüller, Andre Schneider, Hannes Rotzinger, Martin Weides, and Alexey V. Ustinov — Physikalisches Institut, Karlsruhe Institute of Technology

Due to their intrinsic coherence and easy accessibility, superconducting circuits are a promising platform for building a universal quantum computer. Such devices could solve virtually any quantum problem, however many qubits are required in order to achieve quantum supremacy. A more direct, alternative approach is provided by analog quantum simulation. By synthesizing the Hamiltonian of a quantum system with a simulator, the eigenstates and time evolution are investigated without accessing the original system.

In this work, we explore the properties of two coupled concentric transmon qubits. We show strong XX-interaction with a coupling strength of 12 MHz between the qubits. This value is extracted from spectroscopy measurements and confirmed by vacuum Rabi oscillations, in good agreement with electrodynamic calculations.

These results pave way towards future experiments on the quantum dynamics of larger systems with multiple artificial quasi-spins. The concentric transmon is expected also to feature ZZ-coupling, when biased at frequencies away from the flux sweet spot. Depending on the accessible parameter range, the simulation of the Fermi-Hubbard model is offered by a theoretical model. In this contribution, we will show our experimental and numerical data and provide an outlook on performing quantum simulation with concentric transmon qubits.

TT 38.9 Wed 11:45 HSZ 03

Probing the strong coupling regime between microwave resonators and YPc_2 molecule ensembles — •Yannick Schön[1], Eufemio Pineda[2], Hannes Rotzinger[1], Marco Pfirrmann[1], Andre Schneider[1], Julius Krause[1], Sebastian T. Skacel[1], Mario Ruben[2], Alexey V. Ustinov[1], and Martin Weides[1,3] — [1]Karlsruhe Institute of Technology, Institute of Physics — [2]Karlsruhe Institute of Technology, Institute of Nanotechnology — [3]Johannes Gutenberg-University Mainz, Institute of Physics

We investigate magnetic molecule ensembles with microwave signals in the low GHz range. This offers a measurement and manipulation framework, which can reliably be integrated into hybrid quantum systems, and facilitates joint applications of magnetic molecules in the rapidly growing field of quantum information processing.

The studied material family of lanthanide or metal Phtalocyanine 2 compounds exhibits a wide range of splittings between their electronic states, as well as molecular anisotropy, depending on the central ion. Our setup facilitates probing dynamics of different molecules with a 3d cavity in dependence of temperature, power or magnetic field.

In particular, the strong coupling of Yttrium Pc2 (YPc_2) to microwave resonators has been investigated between 25 mK and 20 K, and compared to simulation based on input-output theory. The extracted parameters contain information about the sample transitions, their linewidth, and coupling strength down to the quantum regime. Furthermore, on-chip integration of molecule ensembles with superconducting niobium 2d resonators is demonstrated.

TT 38.10 Wed 12:00 HSZ 03

A pulsed electron paramagnetic resonance spectrometer operating at millikelvin temperatures — •Stefan Weichselbaumer[1,2], Christoph W. Zollitsch[1,2], Kai Müller[1,2], Petio Natzkin[1,2], Sebastian T. B. Goennenwein[1,2,3], Martin S. Brandt[2,4], Rudolf Gross[1,2,5], and Hans Huebl[1,2,5] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Institut für Festkörperphysik, Technische Universität Dresden, Dresden, Germany — [4]Walter Schottky Institut, Technische Universität München, Garching, Germany — [5]Nanosystems Initiative Munich, Munich, Germany

Electron paramagnetic resonance (EPR) is an ubiquitous spectroscopy tool which is employed in many areas of research. One critical aspect for any application is the sensitivity of the spectrometer which scales with the degree of spin polarization in the sample. In the paramagnetic case, this spin polarization is determined by the ratio of magnetic field and temperature, B/T. Here, we report on the implementation of a pulsed EPR spectrometer using superconducting microwave resonators, operating at millikelvin temperatures. We investigate a spin ensemble of phosphorus donors embedded in an isotopically purified nuclear spin free ^{28}Si environment, which exhibits a thermal spin polarization close to unity at 50 mK. Our high sensitivity allows for single-shot measurements with an exceptional signal-to-noise ratio SNR $\gg 1$ for approximately 10^8 spins.

This work was supported by the DFG via SPP 1601 (HU1861/2-1).

TT 38.11 Wed 12:15 HSZ 03

Engineering the parity of light-matter interaction in superconducting circuits — •J. Goetz[1], C. Besson[1,2], P. Eder[1,2,3], M. Fischer[1,2,3], S. Pogorzalek[1,2,3], E. Xie[1,2,3], K.G. Fedorov[1,2], F. Deppe[1,2,3], A. Marx[1], 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

In physics, parity describes the symmetry properties of quantum states and operators under spatial inversion. It has manifold applications in the standard model, quantum information and field theory. We present a novel technique for the in-situ control of the interaction operator

parity in superconducting quantum circuits. Using a tunable-gap gradiometric flux qubit, which exhibits both a dipole and a quadrupole moment, we can precisely engineer the interaction parity with spatially shaped microwave fields. Our highly symmetric sample architecture enables a complete parity inversion and the observation of transparency induced by longitudinal coupling. In a second step, we couple the qubit to a resonator and, in this way, activate quadrupolar transitions similar to those in multi-electron atoms. Our work paves the way towards parity based quantum simulation and physical applications based on longitudinal light-matter interaction.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria, and the IMPRS 'Quantum Science and Technology'.

TT 38.12 Wed 12:30 HSZ 03

Near quantum-limited amplification and conversion based on a voltage-biased Josephson junction — •Salha Jebari[1,2], Florian Blanchet[1,2], Romain Albert[1,2], Dibyendu Hazra[1,2], and Max Hofheinz[1,2] — [1]CEA, Grenoble,France — [2]Université Grenoble Alpes, Grenoble, France

Recent experiments with superconducting circuits consisting of a DC voltage-biased Josephson junction in series with a resonator have shown that a tunneling Cooper pair can emit one or several photons with a total energy of 2e times the applied voltage. We present microwave reflection measurements on the device in , indicating that amplification is possible with a simple DC voltage-biased Josephson junction. We also show that this amplification adds noise close to the limit set by quantum mechanics for phase preserving amplifiers. For low Josephson energy, transmission and noise emission can be explained within the framework of P(E) theory of inelastic Cooper pair tunneling and are related to the fluctuation dissipation theorem (FDT). We also experimentally demonstrate, by controlling the applied DC voltage, that our device can act as both an amplifier and a frequency converter. Combined with a theoretical model, our results indicate that voltage-biased Josephson junctions might be useful for amplification near the quantum limit, being powered by simple DC voltage and providing a different trade-off between gain, bandwidth and dynamic range, which could be advantageous in some situations.

TT 38.13 Wed 12:45 HSZ 03

Josephson-photonics devices as source of non-classical microwave radiation — •Björn Kubala[1], Joachim Ankerhold[1], Chloe Rolland[2], Marc P. Westig[2], Iouri Moukharski[2], Daniel Esteve[2], and Fabien Portier[2] — [1]Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany — [2]CEA Saclay, Gif-sur-Yvette, France

Sources of non-classical photons have important applications in quantum communication and sensing technologies. With non-classical microwave sources these are extended to circuit-QED setups extensively used for various quantum information tasks.

Here, we report recent experimental result, demonstrating that a dc-biased Josephson junction embedded in a carefully engineered electromagnetic environment constitutes a new source of bright non-classical radiation. We will explain, why in such a "Josephson-photonics" device with a single mode of large impedance strongly anti-bunched photons are produced, opening the path to a single-photon source in the microwave range. A Cooper-pair crossing a junction, which is coupled to two resonators, under the proper dc-bias emits a pair of photons into the two resonators and thus produces correlated light with strongly reduced noise [1]. Measurements of this noise reduction factor demonstrate the non-classical nature of the light source.

[1] A. D. Armour, B. Kubala, and J. Ankerhold, Phys. Rev. B **91**, 184508 (2015)

TT 39: Superconductivity: (General) Theory

Time: Wednesday 9:30–13:15 Location: HSZ 103

TT 39.1 Wed 9:30 HSZ 103

Induced Superconductivity in the Hubbard model — •Nikolaj Bittner[1], Takami Tohyama[2], and Dirk Manske[1] — [1]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]Department of Applied Physics, Tokyo University of Science, Tokyo 125-8585, Japan

Recent development of optical pulses at THz and mid-infrared frequencies has reported indications of photo-induced superconductivity at temperatures much higher than superconducting transition temperature (Tc) in cuprate superconductors [1] and K-dopes C_{60} [2]. These are now a hot topic in the field of superconductivity.

In this contribution we present a theoretical study of the nonequilibrium dynamics in the one-dimensional extended Hubbard model at half filling. Particular emphasizes is on the possibility to induce superconductivity in this system driven out of equilibrium. Within the framework of the time-dependent Lanczos algorithm the time evolution of the Hubbard model is investigated for two different nonequilibrium scenarios, which occur by (i) an interaction quench and by (ii) action of a light pulse. For both cases the time dependent optical conductivity and the superconducting correlation functions are calculated. In particular, it was observed from these calculations appearance of a transient Meissner effect, which is a fingerprint of the induced superconductivity. This is in agreement with the obtained correlation functions and opens a new way to induce superconductivity in an experiment.

[1] S. Kaiser et al. PRB, 89, 184516 (2014);
D. Fausti et al. Science 331, 189 (2011)
[2] M. Mitrano et al. Nature, 530, 461 (2016)

TT 39.2 Wed 9:45 HSZ 103

Plaquette valence bond theory of high-temperature superconductivity — •Malte Harland[1], Mikhail I. Katsnelson[2], and Alexander I. Lichtenstein[3] — [1]Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany — [2]Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525AJ Nijmegen, The Netherlands — [3]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, Hamburg 22761, Germany and Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany

We present a strong-coupling approach to the theory of high-temperature superconductivity based on the observation of a quantum critical point in the plaquette within the t, t' Hubbard model. The crossing of ground state energies in the $N = 2, 3, 4$ sectors occurs for parameters close to the optimal doping. The theory predicts the maximum of the $d_{x^2-y^2}$-wave order parameter at the border between localized and itinerant electron behavior and gives a natural explanation for the pseudo-gap formation via soft-fermion mode related to local singlet states of the plaquette in the environment. Our approach follows the general line of resonating valence bond theory stressing a crucial role of singlets in the physics of high-T_c superconductors, but focuses on the formation of *local* singlets.

TT 39.3 Wed 10:00 HSZ 103

The T-dependence of the scattering rate in cuprates: Insights from diagrammatic extensions of DMFT — •Marie-Therese Philipp[1,2], Georg Rohringer[2], Clemens Watzenböck[1], Thomas Schäfer[1], Hartmut Hafermann[3], Jan M. Tomczak[1], Karsten Held[1], Alexey Rubtsov[2], and Alessandro Toschi[1] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Russian Quantum Center, Novaya street, 100, Skolkovo, Moscow region 143025, Russia — [3]Mathematical and Algorithmic Sciences Lab, France Research Center, Huawei Technologies Co. Ltd., 92100 Boulogne-Billancourt, France

We analyze here some of the most recent experimental results[1] for the resistivity ρ and the Hall-resistivity ρ_H of the high-T_c superconducting cuprates. Surprisingly, the measured ratio ρ/ρ_H shows a universal, Fermi-liquid (FL) temperature dependence across the whole phase diagram. In the simplest Drude picture, this ratio would correspond to FL scattering rate ($\gamma \propto T^2$). In this context, γ can be computed in many-body theory from the imaginary part of the self-energy at the Fermi surface $[-Im(\Sigma(w = 0, k_F))]$. In particular, to estimate $-Im(\Sigma(w = 0, k_F))$, we have employed diagrammatic extensions of DMFT, namely the dual fermion (DF) approach and the dynamical vertex approximation (DΓA). The obtained temperature dependences will be compared to a more precise, but also challenging, direct esti-

mate of ρ/ρ_H, by means of the *bubble-like* term of the corresponding conductivity tensors.

[1] N. Barišić, et al. (2015) arXiv:1507.07885

TT 39.4 Wed 10:15 HSZ 103

Charge and current orders in the cuprates: implications from spin-fermion model with overlapping hot spots. — •Pavel A. Volkov and Konstantin B. Efetov — Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Experiments carried over the last years on the underdoped cuprates suggest the presence of a variety of symmetry-breaking phenomena in the pseudogap phase. Charge-density waves, breaking of C_4 rotational symmetry, as well as time-reversal symmetry breaking have all been observed in several cuprate families. Unification of these phenomena thus poses a crucial theoretical challenge. We address this issue in the framework of the spin fluctuation scenario, where the low-energy fermions interact through the exchange of antiferromagnetic fluctuation quanta, paramagnons. We study particle-hole instabilities in a model explicitly taking into account two regions of the Fermi surface: around $(0,\pi)$ and $(\pi,0)$. For a quasi-1D dispersion in both regions, we show that for sufficiently small $|\varepsilon(\pi,0)-E_F|$, the leading instability is a d-form factor Fermi surface deformation (Pomeranchuk instability). It naturally produces a C_4-breaking and supports the formation of a unidirectional bond-oriented d-form factor CDW at lower temperatures, consistent with experiments. Additionally, we show that the Fermi surface curvature in the antinodal regions promotes a state formed by current loops organized in an antiferromagnetic structure (as in the d-density wave state), and thus breaking time-reversal symmetry.

TT 39.5 Wed 10:30 HSZ 103

Three-band superconductors with broken time reversal symmetry ground states — •Yuriy Yerin[1,2], Alexander Omelyanchouk[2], Stefan-Ludwig Drechsler[3], Jeroen van den Brink[3], and Dmitri Efremov[3] — [1]Institute for Physics of Microstructures, Russia — [2]Institute for Low-Temperature Physics , Ukraine — [3]Institute for Theoretical Solid State Physics, Leibnitz Institute IFW-Dresden, Germany

Within the Ginzburg-Landau formalism we provide a classification of all possible ground states of a three-band superconductor (SC) where either states with broken time-reversal symmetry (BTRS) or a single non-BTRS ground state of s-wave symmetry are realized. We track possible evolutions of the BTRS ground state in an external magnetic field. We show that an external magnetic field may trigger transitions between BTRS and non-BTRS states. We propose to use the current induced magnetic flux response of samples with a doubly-connected geometry as a suitable experimental searching method for the detection of BTRS ground states as well as of corresponding metastable excited state in three-band SC. The latter can be involved in a flux regime nonadiabatically switched on. Due to frustration of the three-band order parameter components topological solitons and other inhomogeneous topological states are possible and will be briefly discussed, too.

TT 39.6 Wed 10:45 HSZ 103

f-wave triplet superconductivity in a twisted triangular Hubbard tube as a model of $A_2Cr_3As_3$ — Sahinur Reja[1] and •Satoshi Nishimoto[2,3] — [1]Indiana University, Bloomington, USA — [2]TU Dresden, Germany — [3]IFW Dresden, Germany

Triplet superconductivity (SC) recently has been one of the active research topics partly due to its intrinsic connection to quantum computations. In this contex, we study the ground state properties of a twisted triangular Hubbard tube using the perturbation theory and density-matrix renormalization group method. We show that two electrons in an odd-site Hubbard ring always form a spin-triplet pair, and subsequently a polarized ferromagnetic (FM) order is stabilized in a wide range of electron filling (n) when these rings are weakly coupled. By calculating the binding energy and spin gap, we confirm the presence of the spin-triplet SC after melting of the FM order with increasing the inter-triangle couplings (t_2). We show that triplet SC pair correlations are consistent with the f-wave channel. We present a detailed n-t_2 phase diagram which features also singlet SC at $n \sim 1$ and $t_2 \sim 1$. Finally we argue that this model has possible relevance to the f-wave SC observed in alkali chromium arsenides $A_2Cr_3As_3$ (A=K,Rb,Cs).

TT 39.7 Wed 11:00 HSZ 103

Inflated nodes in multiband superconductors with broken time-reversal symmetry — •Carsten Timm[1], Daniel F. Agterberg[2], and Philip M. R. Brydon[3] — [1]Institute of Theoretical Physics, Technische Universität Dresden, Germany — [2]Department of Physics, University of Wisconsin, Milwaukee, U.S.A. — [3]Department of Physics, University of Otago, Dunedin, New Zealand

It is commonly believed that superconductors fall into one of three classes: They can have a full energy gap, a gap with point nodes, or a gap with line nodes. We show that multiband, even-parity, nodal superconducting states that break time-reversal symmetry do not belong to these classes. Instead, they *generically* possess two-dimensional Fermi surfaces. These Fermi surfaces can be visualized as being generated by "inflating" point and line nodes into spheroids and tori, respectively. The inflated nodes are topologically protected by a $\mathbb{Z}_2$ invariant, which we give in terms of a Pfaffian. We also show that such states can be *energetically* stable in spite of the extended Fermi surfaces; they form the state with the lowest free energy if spin-orbit coupling is sufficiently strong.

15 min. break.

TT 39.8 Wed 11:30 HSZ 103

Mutually attracting spin waves in the square-lattice quantum antiferromagnet — •Kai Phillip Schmidt[1], Michael Powalski[2], and Götz S. Uhrig[2] — [1]FAU Erlangen-Nürnberg, Erlangen, Germany — [2]TU Dortmund, Dortmund, Germany

Spin waves (magnons) in two dimensions are the potential glue in high-temperature superconductors so that their quantitative understanding is mandatory. Yet even for the fundamental case of the undoped Heisenberg model on the square lattice a consistent picture is still lacking. Significant spectral continua are taken as evidence of the existence of fractional excitations (spinons), but descriptions in terms of spinons fail to show the established absence of an energy gap. Here a fully consistent picture of the dynamics of magnetism in the square-lattice quantum antiferromagnet is provided which agrees with the experimental findings. The key step is to capture the strong attractive interaction between the spin waves.

TT 39.9 Wed 11:45 HSZ 103

Ab-initio characterization of superconductivity in the elemental phases of phosphorus: from black-P up to 350 GPa — •Antonio Sanna[1], Jose Flores-Livas[2], Gianni Profeta[3], and Lilia Boeri[4] — [1]MPI for Microstucture Physics, Halle, Germany — [2]University of Basel, Switzerland — [3]University of L'Aquila, L'Aquila, Italy — [4]TU Graz, Austria

We present the result of a complete ab-initio characterization of elemental phosphorus in its structural and superconducting properties.

At low pressure we discuss the possibility of superconductivity in Black-P upon doping. In the high pressure regime we investigate thermodynamic stability by performing structural search with the minima hopping method. This way identifying structures that are likely to form upon compression. On the low enthalpy structures we perform full electronic and phononic characterization within DFT-PBE. Superconducting properties are predicted by means of Density Functional Theory for Superconductors.

Apart from several interesting predictions, calculations provide a nice interpretation of the existing experimental data, in particular of the evidence that different experimental procedures lead to significantly different values of the critical temperature.

TT 39.10 Wed 12:00 HSZ 103

First principles based proximity effect of superconductor-normal metal heterostructures — •Gabor Csire[1], Balazs Ujfalussy[1], and Jozsef Cserti[2] — [1]Wigner RCP, Budapest, Hungary — [2]Eotvos University, Budapest, Hungaty

We investigate the proximity effect in superconductor-normal metal heterostructures based on first principles calculations with treating the pairing potential as an adjustable parameter. The superconducting order parameter (anomalous density) is obtained from the Green-function by solving the Kohn-Sham-Bogoliubov-de Gennes equations with the Screened Korringa-Kohn-Rostoker method. The results are interpreted for an Au/Nb(001) system. The layer resolved anomalous spectral function is also obtained which is closely related to the superconducting order parameter. We show that the proximity effect can be understood via the anomalous spectral function.

TT 39.11 Wed 12:15 HSZ 103

Friedel-oscillations in inhomogeneous topological superconductors — •Lars Lauke[1], Mathias Scheurer[1], Andreas Poenicke[1,2], and Jörg Schmalian[1] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Deutschland — [2]Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Deutschland

In order to investigate Majorana bound states in p-wave superconductors and to reveal the precise influence of boundaries and inhomogeneities on the local structure of competing superconducting order parameters, we solve inhomogeneous Bogoliubov-de Gennes equations. Going beyond the quasi-classical approach we examine in particular the role of Friedel-oscillations due to inhomogeneities and the surface of the superconductor and analyse the distinct behaviour of the p-wave and the surface induced s-wave pairing amplitudes.

TT 39.12 Wed 12:30 HSZ 103

Exotic vortex configurations and superconductors with shallow bands — •Sebastian Wolf[1], Alexei Vagov[1], Arkady Shanenko[2], José Albino Aguiar[2], and Vollrath Martin Axt[1] — [1]Institut for Theoretical Physics III, University Bayreuth, Germany — [2]Departamento de Física, Universidade Federal de Pernambuco, Recife, Brazil

Experiments revealed that the magnetic response of superconducting materials that are close to the interchange between type I and type II may be very different from either of the two standard types [1,2]. The interval of such non-conventional behavior, referred to as the inter-type superconductivity, is rather small in traditional materials but can be considerably enlarged in non-conventional multi-band superconductors such as in MgB_2 [2]. Theoretical description of this interval requires an approach beyond the traditional Ginzburg-Landau theory. In our work we investigate inter-type superconductors within the framework of the extended Ginzburg-Landau theory [3].

Using this approach we demonstrated a general enlargement tendency for the inter-type domain in multi-band superconductors, especially when one of the contributing bands is shallow. In order to explain the appearance of non-conventional mixed states we studied details of the vortex-vortex interaction, in particular the crossover between the monotonic and the non-monotonic interaction.

[1] U. Krägeloh, Physics Letters A **28**, 657-658 (1969)
[2] V. Moshchalkov et al., Phys. Rev. Lett. **102**, 117001 (2009)
[3] A. V. Vagov et al., Phys. Rev. B **85**, 014502 (2012)

TT 39.13 Wed 12:45 HSZ 103

Exploring the Efimov effect in conventional superconductors — •Ali Sanayei[1], Pascal Naidon[2], and Ludwig Mathey[1] — [1]Center for Optical Quantum Technologies, Institute for Laser Physics, University of Hamburg, Luruper Chaussee 149, D-22761 Hamburg — [2]RIKEN Nishina Centre, RIKEN, Wako 351-0198, Japan

In this work, we explore the emergence of the Efimov effect in solid state physics. We consider a three-electron system in distinguishable states of (band 1, up), (band 2, up), and (band 2, down) in a solid. The electron in band 1 is located in an otherwise empty band and interacts through a spin-independent interaction with the two up- and down-electrons in band 2, both of which are immersed in a Fermi sea. Introducing a proper renormalization of the coupling constants, we derive a system of two coupled integral equations describing a three-electron eigenstate in momentum space. These equations support a trimer state solution of electrons, which is a demonstration of the Efimov effect in conventional superconductors.

TT 39.14 Wed 13:00 HSZ 103

Multi-particle instability in an imbalanced electron gas — •Gareth Conduit and Thomas Whitehead — Department of Physics, University of Cambridge, UK

We show that in an imbalanced electron gas weak attractive interactions induce a multi-particle instability, binding multiple electrons together. The maximum binding energy per particle is achieved where the ratio of the number of up/down spin particles in the instability is equal to the ratio of the up/down spin density of states. We use this instability to propose a new superconducting ground state that has lower energy than the FFLO state.

TT 40: Transport: Molecular Electronics and Photonics (jointly with CPP, HL, MA, O)

Time: Wednesday 9:30–12:45 Location: HSZ 201

TT 40.1 Wed 9:30 HSZ 201

Negative differential conductance in single-molecule junctions with ferromagnetic electrodes — •Peter Hasch, Yuxiang Gong, Li Jiang, Carlos-Andres Palma, Joachim Reichert, and Johannes V. Barth — Physics Department E20, Technische Universität München, Germany

Scaling down logic operations to the level of single molecules might be considered the next frontier in computation. One approach is to electrically control single spin states in a molecule, trapped between two electrodes.

Here we report the observance of a negative differential conductance (NDC), measured in a single-molecule junction. The investigated NDC could be explained by a single-spin phenomenon, arising when the molecule gets charged due to voltage-induced depopulation of the highest occupied molecular orbital. This oxidation is monitored by Raman spectroscopy, which allows to analyze chemical and electronical structures with a single-molecule sensitivity. By (anti)ferromagnetic coupling of the unpaired spin on the molecule to one of the electrodes, the molecule might act as a spin-valve, blocking charge transport of the opposite spin direction.

Single-molecule NDC elements bear considerable potential for logical crossbar architectures, and could shrink the actual state of the art devices significantly in size.

TT 40.2 Wed 9:45 HSZ 201

Single-molecule junctions with oligoynes and epitaxial graphene nanoelectrodes — •Konrad Ullmann[1], Susanne Leitherer[2], Maximilian Krempe[3], Rik Tykwinski[3], Michael Thoss[2], and Heiko Weber[1] — [1]Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [3]Organische Chemie I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Single molecule junctions using graphene as electrode material have drawn considerable attention in recent years [1,2]. Due to their open access architecture, their transparency and robustness, they are well suited for a variety of unprecedented experiments. The electrode material graphene also allows for new anchor groups which connect the molecule to the electrode, e.g. via Pi-interaction.

We report on experiments using an oligoyne molecular wire with platinum termination, being contacted with epitaxial graphene nanoelectrodes. I-V characteristics show a linear behavior with a conductance close to the conductance quantum. Furthermore we present an experimental setup which uses electrospray ionisation to bring the molecules in contact with the graphene electrodes.

[1] K. Ullmann et al., Nano Lett. 15, 3512, 2015
[2] F. Prins et al., Nano Lett. 11, 4607, 2011

TT 40.3 Wed 10:00 HSZ 201

Visualizing the role of molecular orbitals in charge transport through individual diarylethene Isomers — •Gaël Reecht[1], Christian Lotze[1], Dmytro Sysoiev[2], Thomas Huhn[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin , Berlin ,Germany — [2]Universität Konstanz, Konstanz, Germany.

Diarylethene molecules are prototype molecular switches with their two isomeric forms exhibiting strikingly different conductance, while maintaining similar length. With a scanning tunneling microscope (STM) we investigate the electronic structure and the transport properties of the open and closed isomers of a sulfur-free diarylethene. The electronic structure is determined with scanning tunneling spectroscopy (STS) for the molecule lying on the surface. Between the two isomers, intriguing differences of the energy and the spatial extend of the molecule orbitals are observed. We then lift the two isomers with the tip of the STM and measure the current passing through the individual molecules. We observe an important difference of conductance between the two forms. With a simple analytical model of transport

based on the results of the STS measurements, we show that the previously determined orbital characteristics are essential ingredients for the complete understanding of the transport properties.

TT 40.4 Wed 10:15 HSZ 201

Electronic transport properties of a tripodal molecular platform — •Safa Golrokh Bahoosh, Amin Karimi, Elke Scheer, and Fabian Pauly — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Intensive studies on single-molecule junctions have been performed to explore the implementation of molecular-scale devices and to understand how the molecules transport charges[1]. While molecules with delocalized π-systems are the ideal compounds to form wires for electronic applications due to their expected high conductance, tripodal molecular platforms that points almost perpendicular to the surface, appear as promising candidates to establish a conducting path between two electrodes. To take into account these aspects, a 9,9'-spirobifluorene (SBF) platform has been introduced. By combining experimental and theoretical investigations of elastic and inelastic charge transport, we show that the current proceeds through the molecular "backbone" and identify a binding geometry that is compatible with the experimental observations in mechanically controlled break junctions[2]. The conductive molecular wire on the platform features a well-defined and relatively high conductance despite the length of the current path of more than 1.7 nm. If time permits, the possibility to use these molecules as a molecular toggle switch, as observed in subsequent studies with a scanning tunneling microscope, will be discussed.

[1] S. Aradhy, and L. Venkataraman, Nature Nanotechnol. 8, 399 (2013)
[2] M. A. Karimi, S. G. Bahoosh, M. Valášek, M. Bürkle, M. Mayor, F. Pauly, and E. Scheer, Nanoscale 8, 10582 (2016)

TT 40.5 Wed 10:30 HSZ 201

Analysis of local current through molecular wires in open quantum systems — •Daijiro Nozaki, Andreas Lücke, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany

The understanding of the local electronic flows in single molecules is of fundamental importance in the design of functional molecules as well as molecule-based electronic devices [1-4]. The charge transport through molecular wires connected between contacts is investigated using non equilibrium Green's function formalism combined with Landauer formula. Energy-dependent and total current through a series of molecular junctions are calculated in real space representation. The influence of contact positions, functional groups, and the replacement of atoms as defects on the transport properties are examined systematically. The static current-induced local magnetic field is also investigated in carbon-based molecular wires. It is shown that even in the same bias directions the direction of the magnetic field is easily reversed depending on the molecular topologies and the positions of electric contacts.

[1] M. Walz, J. Wilhelm, and F. Evers Phys. Rev. Lett. **113**, 136602 (2014)
[2] J. Wilhelm, M. Walz, and F. Evers Phys. Rev. B **92**, 014405 (2015)
[3] G. C. Solomon, C. Herrmann, T. Hansen, V. Mujica, and M. A. Ratner Nat. Chem. **2**, 223 (2010)
[4] T. Ono and K. Hirose, Phys. Rev. Lett. **98**, 026804 (2007)

TT 40.6 Wed 10:45 HSZ 201

Controlling the conductance of graphene-molecule junctions by proton transfer — •Dominik Weckbecker, Pedro B. Coto, and Michael Thoss — FAU Erlangen-Nürnberg, Institut für Theoretische Physik, Staudtstrasse 7/B2, 91058 Erlangen, Germany

The possibility of using single-molecule junctions as components of nanoelectronic devices has motivated intensive experimental and theoretical research on the underlying transport mechanism in these systems [1]. In this contribution, we investigate from a theoretical perspective intramolecular proton transfer reactions as a mechanism for controlling the conductance state of graphene-based molecular junctions. Employing a methodology that combines first-principles electronic structure calculations with nonequilibrium Green's function transport theory [1], we show that the proton transfer reaction proceeds via a two-step mechanism and gives rise to several states of the junction with different conductance properties. In addition, we demonstrate that the relative stability of the different conductance states and the energy barriers for the interconversion reactions can be controlled by means of an external electrostatic field. The possibility of using this mechanism for the design of nanomolecular devices such as diodes or switches is also discussed [2,3].

[1] Cuevas, J. C. and Scheer, E., Molecular Electronics, World Scientific Pub. Co., Singapore, 2010
[2] Hofmeister, C. *et al.*, J. Mol. Model. **20**, 2163 (2014)
[3] Hofmeister, C. *et al.*, arXiv: 1611.01027v1 (2016)

15 min. break.

TT 40.7 Wed 11:15 HSZ 201

Hierarchical Quantum Master Equation Approach to Vibrationally Coupled Nonequilibrium Charge Transport in Single-Molecule Junctions — •Christian Schinabeck[1], André Erpenbeck[1], Rainer Härtle[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany. — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen, 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 perturbative master equations. We demonstrate the importance of vibrational nonequilibrium effects for a model molecular junction consisting of an electronic level coupled to fermionic leads as well as a vibrational mode. In particular, in the off-resonant transport regime, the inelastic cotunneling signal is analyzed for a vibrational mode in full nonequilibrium, revealing a complex interplay of different transport processes and deviations from the commonly used $G_0/2$ rule of thumb [3]. Moreover, an extension of the HQME approach is presented, which allows the calculation of the full counting statistics. Using this method, the influence of higher-order cotunneling processes on the current fluctuations is analyzed.

[1] Y. Tanimura *et al.*, J. Phys. Soc. Jpn. **75**, 082001 (2006).
[2] J. Jin *et al.*, J. Chem. Phys. **128**, 234703 (2008).
[3] C. Schinabeck *et al.*, Phys. Rev. B **94**, 201407 (2016).

TT 40.8 Wed 11:30 HSZ 201

Theoretical study of current-induced bond rupture in molecular junctions — •André Erpenbeck, Christian Schinabeck, Lukas Götzendörfer, 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

Electronic-vibrational coupling in charge transport through single molecule junctions may result in current-induced bond rupture and is thus an important mechanism for the stability of the junction. In this contribution, we demonstrate how the hierarchical quantum master equation (HQME) theory in combination with the quasi-classical Ehrenfest approach for the nuclear degrees of freedom can be used to simulate current-induced bond rupture in single molecule junctions. Employing generic models for molecular junctions with dissociative nuclear potentials, we analyze the underlying mechanisms. In particular, we investigate the dependence of the current, the population and the dissociation probability on the model parameters. In addition, we validate the quasi-classical Ehrenfest approach using numerically exact results obtained by the HQME method [1] for a model comprising one harmonic vibrational mode.

[1] C. Schinabeck, A. Erpenbeck, R. Härtle, M. Thoss, Phys. Rev. B 94, 201407(R) (2016)

TT 40.9 Wed 11:45 HSZ 201

Spin Transport in Helical Systems — •Matthias Geyer[1,2], Rafael Gutiérrez[1], Stefan Siegmund[3], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany — [3]Center for Dynamics, TU Dresden, 01062 Dresden, Germany

Various experiments have shown strong spin selectivity in chiral molecules like DNA at room temperature. Since atomic spin orbit coupling alone is insufficient to explain the effect's magnitude, a relation to the helical geometry has been suggested. We want to provide a better understand of the underlying mechanisms by analytically and numerically investigating suitable models for electrons in helical systems with spin orbit coupling.

We follow two complementary approaches: a generic and simplified model to study the bare influence of the helical geometry and a more

realistic one to calculate the effect for specific molecules. The former starts with a 3D continuum model with helix-shaped confinment from which an effective 1D Hamiltonian is derived using adiabatic perturbation theory. For the ladder an effective tight-binding model is derived from the microscopic Hamiltonian of a specific molecule. Incoherent transport calculations are performed for both models using master equations with dephasing, accounting for decoherence due to the coupling to vibrational degrees of freedom arising from structural fluctuation.

TT 40.10 Wed 12:00 HSZ 201

Charge Carrier Dynamics in κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl: From Mott Insulator to Quantum Spin Liquid — •Jana-Isabelle Polzin[1], Benedikt Hartmann[1], Takahiko Sasaki[2], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, Germany — [2]Institute for Materials Research, Tohoku University, Sendai, Japan

The organic charge transfer salts κ-(ET)$_2$X are model systems for studying strongly-correlated charge carriers and the Mott metal-insulator transition in reduced dimensions. Recently, the influence of quenched disorder attracted considerable attention. Conducting layers of ET molecules are separated by thin, insulating sheets with anions X, resulting in a quasi-2D electronic band structure. Within the ET layers the molecules are arranged in dimers forming a triangular lattice. One free charge carrier exists per dimer, its spin being geometrically frustrated. The Mott insulator κ-(ET)$_2$Cu[N(CN)$_2$]Cl shows antiferromagnetic ordering at $T_N \approx 27\,K$. It has been shown that increasing disorder induced by X-ray irradiation drives the Mott insulating state with long-ranged antiferromagnetic order into a quantum spin liquid state [1]. Here, we discuss comparative measurements of fluctuation spectroscopy on pristine and irradiated samples in order to investigate the changes in electronic transport mechanism and low-frequency charge carrier dynamics [2] when tuning the Mott insulator to the spin liquid ground state. This results in a decrease of both resistivity and the current or voltage fluctuations after irradiation.

[1] PRL 115, 077001 (2015)
[2] PRL 114, 216403 (2015)

TT 40.11 Wed 12:15 HSZ 201

Charge Carrier Dynamics at the Mott transition in κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br — •Tatjana Thomas[1], Benedikt Hartmann[1], Takahiko Sasaki[2], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, Germany — [2]Institute for Materials Research, Tohoku University, Sendai, Japan

The organic charge transfer salts κ-(ET)$_2$X are considered as model systems for studying the Mott metal-insulator transition – a key phenomenon in the physics of strongly correlated electrons – in reduced dimensions. In particular, the influence of disorder on the criticality of the Mott transition recently has been a matter of debate. Partially deuterated κ-[(H$_8$-ET)$_{0.2}$(D$_8$-ET)$_{0.8}$]$_2$Cu[N(CN)$_2$]Br, which is located in the critical region of the phase diagram, can be fine-tuned through the Mott transition by utilizing a glass-like structural ordering transition of the ET molecules' terminal ethylene groups. By applying different thermal relaxation protocols, both the ratio of W/U and a small degree of quenched disorder can be set at will, the former corresponding to changes in hydrostatic pressure of ~ 200 bar. We employ fluctuation (noise) spectroscopy as a powerful tool to study the charge carrier dynamics at low frequencies. When crossing the S-shaped Mott transition line, surprisingly we observe a step-like increase of the resistance fluctuations in the metallic region. We discuss our results in terms of critical slowing down of the order parameter fluctuations [1] and electronic phase separation, and an extended region of the phase diagram where the fluctuations are non-Gaussian.

[1] B. Hartmann et al., *Phys. Rev. Lett.* **114**, 216403 (2015).

TT 40.12 Wed 12:30 HSZ 201

Thermal conductance of Teflon and Polyethylene: Insight from an atomistic, single-molecule level — •Marius Buerkle and Yoshihiro Asai — AIST, Tsukuba, Japan

The thermal transport properties of teflon (polytetrafluoroethylene) and its polyethylene counterparts are, while highly desirable and widely used, only superficially understood. Here, we aim therefore to provide rigorous insight from an atomistic point of view in context of single-molecule devices. We show that for vinyl polymers adsorbed on metal-surfaces the thermal transport strongly depends one the properties of the metal-molecule interface and that the reduced thermal conductance observed for teflon derivatives originates in a reduced phonon injection life time. In asymmetric molecules phonon blocking on the intra molecular interface leads to a further reduction of thermal conductance. For hetrojunctions with different electrode materials we find that thermal conductance is suppressed due to a reduced overlap of the available phonon modes in the different electrodes. A detailed atomistic picture is thereby provided by studying the transport through perfluorooctane and octane on a single-molecule level using first principles transport calculations and nonequilibrium molecular dynamic simulations.

TT 41: Correlated Electrons: Quantum-Critical Phenomena

Time: Wednesday 9:30–13:00 Location: HSZ 204

TT 41.1 Wed 9:30 HSZ 204

Quantum criticality with a twist: interplay of strong correlations and Kohn anomalies in three dimensions — •Thomas Schäfer[1], Andrey A. Katanin[2], Karsten Held[1], and Alessandro Toschi[1] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Institute of Metal Physics, 620990, Kovalevskaya str. 18, Ekaterinburg, Russia; Ural Federal University, 620002, Mira str. 19, Ekaterinburg, Russia

Quantum critical points (QCPs) are among the most interesting phenomena in condensed matter systems and can emerge by exploiting a non-thermal parameter to suppress finite-temperature phase transitions. Although the limit of zero temperature cannot be reached experimentally, the existence of a QCP can severely influence the system's excitation spectrum. In spite of the intrinsic interest, a consistent theory for QCPs has not been established yet, due to the associated intermingling of temporal and spatial correlations. In this talk, quantum critical properties of the fundamental model of electronic correlations, the Hubbard model in three dimensions, are studied by means of a diagrammatic extension of the dynamical mean field theory, the dynamical vertex approximation (DΓA). The model's magnetic phase diagram is computed upon doping and its critical regions and exponents are analyzed. Quite unexpectedly, the quantum critical properties are found to be driven by the model's Fermi surface properties (Kohn points), even in presence of strong correlations, contradicting the predictions of the conventional Hertz-Millis-Moriya theory.

[1] T. Schäfer et al., arXiv:1605.06355 (2016).

TT 41.2 Wed 9:45 HSZ 204

Critical spin dynamics in YbCo$_2$Si$_2$ — A. Hannaske[1], K. Schmalzl[2], C. Geibel[1], and •O. Stockert[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]JCNS at ILL, Grenoble, France

The strongly correlated compound YbCo$_2$Si$_2$ is the antiferromagnetically ordered sister compound to quantum critical YbRh$_2$Si$_2$. The magnetic order in YbCo$_2$Si$_2$ with $T_N = 1.7$ K can be continuously suppressed upon application of a magnetic field with a critical field of $B_c = 2$ T. We performed detailed inelastic neutron scattering experiments on single-crystalline YbCo$_2$Si$_2$ to study the spin dynamics at B_c. A critical slowing down of the magnetic response is observed as function of temperature at B_c with slightly sublinear temperature dependence of the relaxation rate of the critical spin fluctuations. Moreover, as inferred from measurements at finite momentum transfer, away from the antiferromagnetic ordering wave vector, the paramagnons soften and their lifetime decreases with temperature. Our results will be compared with theoretical calculations.

TT 41.3 Wed 10:00 HSZ 204

Microstructured YbRh$_2$Si$_2$ and YbNi$_4$P$_2$: Magnetoresistance at low temperatures — •Alexander Steppke[1], Sandra Hamann[1], Markus König[1], Andrew P. Mackenzie[1], Kristin Kliemt[2], Cornelius Krellner[2], Heike Pfau[3], Ramzy Daou[4], and Manuel Brando[1] — [1]MPI for Chemical Physics of Solids, Noethnitzer Str. 40, 01187 Dresden — [2]Goethe-Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt am Main — [3]Stanford Institute

for Materials and Energy Science, 2575 Sand Hill Road Menlo Park, California 94025, USA — [4]Normandie Univ, ENSICAEN, CNRS, CRISMAT, 14000 Caen, France

With electrical transport measurements providing valuable information about novel phases or topological changes of the Fermi surface we investigated the properties of $YbRh_2Si_2$ and $YbNi_4P_2$. In the Kondo lattice $YbRh_2Si_2$ the recent discovery of a strong change in the ac susceptibility indicates a superconducting state below 2 mK [1]. Yet data of resistive transitions at these temperatures are still absent, due to the challenge of measuring resistances with minimal dissipation. Furthermore magnetoresistance measurements can be used to detect field induced Lifshitz transitions in both systems. Here we show that by modifying the geometry of clean bulk samples using focused ion beam the resistance can be increased by several orders of magnitude without influencing the magnetic or electronic properties. This opens a path to resistance measurements at ultra low temperatures.

[1] E. Schuberth et al. Science 351, 485 (2016)

TT 41.4 Wed 10:15 HSZ 204

Angle-dependent electron spin resonance measurements on $YbRh_2Si_2$ down to 1.6 K using superconducting planar resonators — •Linda Bondorf[1], Manfred Beutel[1], Markus Thiemann[1], Kristin Kliemt[2], Jörg Sichelschmidt[3], Cornelius Krellner[2], Martin Dressel[1], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Goethe-Universität, Frankfurt am Main, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

$YbRh_2Si_2$ is a tetragonal heavy-fermion system with strong magnetic anisotropy. Its antiferromagnetic order below 70 mK can be suppressed by an in-plane magnetic field of 60 mT, which leads to a quantum critical point. Experimental challenges, e.g. for neutron spectroscopy have so far prohibited a full understanding of the antiferromagnetism of YbRh2Si2. Here, angle-dependent electron spin resonance (ESR) could be an alternative method. However, conventional ESR spectrometers are limited in frequency (typically 9 GHz, corresponding to 200 mT for YbRh2Si2) and temperature (down to 2 K).

To overcome these limitations, we use superconducting planar microwave resonators, and we have performed angle-dependent ESR measurements with in-situ rotation of $YbRh_2Si_2$ single crystals inside a ^{4}He cryostat down to 4.4 GHz and 1.6 K. We present the ESR g-factor as a function of angle, which is consistent with results of previous measurements at higher temperatures and frequencies. Angle-dependent ESR investigations inside the antiferromagnetic phase of $YbRh_2Si_2$ can now be addressed experimentally.

TT 41.5 Wed 10:30 HSZ 204

Grüneisen ratio divergence at the structural quantum critical point in $(Ca_{0.9}Sr_{0.1})_3Rh_4Sn_{13}$ — •Rudra Sekhar Manna[1], Andreas Wörl[1], Swee K. Goh[2], Kazuyoshi Yoshimura[3], and Philipp Gegenwart[1] — [1]EP VI, EKM, Augsburg University, 86159 Augsburg, Germany — [2]Dept. of Physics, The Chinese University of Hong Kong, Hong Kong, China — [3]Dept. of Chemistry, Kyoto University, Kyoto 606-8502, Japan

Quasi-skutterudite compound $Sr_3Rh_4Sn_{13}$ shows a second-order structural phase transition at 138 K which can be tuned to 0 K either by applying hydrostatic pressure or by chemical pressure in $(Ca_xSr_{1-x})_3Rh_4Sn_{13}$. At the critical concentration, $x_c = 0.9$, specific heat shows a pronounced enhancement (compared to the x = 0) of the low-temperature phonon (T^3) contribution, possibly related to the softening of an optical mode [1]. We have performed high-resolution thermal expansion and specific heat measurements on single crystal of x = 0 and a lump of small $(Ca_{0.9}Sr_{0.1})_3Rh_4Sn_{13}$ crystals. Thermal expansion also detects a strongly enhanced phonon contribution at the critical concentration. Importantly, the effective Grüneisen parameter $\Gamma_{eff} = \beta \cdot V_{mol}/\kappa_T \cdot C$ diverges from 20 K down to below 1 K, providing evidence for quantum criticality.

[1] S. K. Goh, D. A. Tompsett, P. J. Saines, H. C. Chang, T. Matsumoto, M. Imai, K. Yoshimura, and F. M. Grosche, PRL **114**, 097002 (2015).

TT 41.6 Wed 10:45 HSZ 204

Magnetic and structural phase transitions in $CeCu_{6-x}Au_x$ — •Sebastian Kuntz[1], Kai Grube[1], Lothar Pintschovius[1], Frank Weber[1], Peter Schweiss[1], Oliver Stockert[2], Veronika Fritsch[3], Sebastian Bachus[3], Yasuyuki Shimura[3], Philipp Gegenwart[3], and Hilbert von Löhneysen[1,4] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, D-76021 Karlsruhe, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, D-01187 Dresden, Germany — [3]Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany — [4]Physikalisches Institut, Karlsruher Institut für Technologie, D-76049 Karlsruhe, Germany

The heavy-fermion compound $CeCu_{6-x}Au_x$ is a model system for unconventional quantum criticality. At small Au contents $CeCu_{6-x}Au_x$ reveals a structural transition from an orthorhombic to a monoclinic crystal symmetry while at higher x an antiferromagnetic phase appears. To shed light on the interplay between quantum critical magnetic and structural fluctuations we performed neutron scattering experiments and thermodynamic measurements on samples with varying Au concentration between $x = 0$ and 0.3. The application of hydrostatic and chemical pressure allows to separate the magnetic from the structural transition and demonstrates that the unconventional quantum criticality is based on the magnetic fluctuations and not influenced by the monoclinic distortion.

TT 41.7 Wed 11:00 HSZ 204

Coherent Emergence of a Quantum Critical Heavy Fermion Groundstate — •Christoph Wetli[1], Johann Kroha[2], Oliver Stockert[3], Hilbert von Löhneysen[4], Kristin Kliemt[5], Cornelius Krellner[5], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zürich — [2]Institute of Physics, Bonn University — [3]MPI for Chemical Physics of Solids, Dresden — [4]Institute of Solid State Physics, KIT — [5]Institute of Physics, Goethe University Frankfurt

Kondo quasiparticles in heavy-fermion metals have an outstandingly long lifetime. However, near a quantum phase transition, the quasiparticles may disintegrate and give way to an exotic state of matter where the very concept of a particle breaks down. We investigate the emergence of this quantum critical behavior in a time-resolved Terahertz reflection experiment. Due to the non-ionizing nature of Terahertz radiation, we directly monitor the formation dynamics of a strongly correlated groundstate in a time-resolved experiment, while simultaneously monitoring the spectral weight and the Kondo temperature. In the quantum critical $CeCu_{5.9}Au_{0.1}$ compound, the heavy-fermion state reconvenes after 5.8 ps under the emission of a temporally delayed, yet phase-coherent reflex. When the temperature is lowered, the changing dynamics indicates the emergence of the unconventional quantum critical state. A decrease in amplitude and an increase in delay of the reflex reveals that the quasiparticle weight collapses while the Kondo temperature reduces but remains finite.

15 min. break.

TT 41.8 Wed 11:30 HSZ 204

Quantum oscillations in the pressure-metallised Mott insulator NiS_2 — •Konstantin Semeniuk[1], Hui Chang[1], Sven Friedemann[2], Jordan Baglo[1], Monika Gamza[3], Pascal Reiss[4], Alix McCollam[5], Inge Leermakers[5], Patricia Alireza[1], Audrey Grockowiak[6], William Coniglio[6], Stanley Tozer[6], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]HH Wills Laboratory, University of Bristol, UK — [3]Jeremiah Horrocks Institute, University of Central Lancashire, UK — [4]Clarendon Laboratory, University of Oxford, UK — [5]High Field Magnet Laboratory, Nijmegen, The Netherlands — [6]NHMFL, Tallahassee, Florida, USA

The metallic state on the threshold of Mott localisation represents one of the most fundamental examples of correlated electron physics. The 3D Mott insulator NiS_2 can be tuned into the metallic state by moderate hydrostatic pressure of about 30 kbar, enabling quantum oscillation measurements in close proximity to the Mott transition.

We present the results of a comprehensive Fermi surface study of NiS_2 performed in magnetic fields of up to 35 T, using a tunnel diode oscillator technique with 0.01ppm frequency resolution in combination with liquid medium high pressure anvil cells. The evolution of the Fermi surface and the effective carrier masses of NiS_2 has been tracked from 33 to 55 kbar, and a rotation study has been carried out to resolve the 3D geometry of the principal Fermi surface sheet. Our results are interpreted in the context of the canonical Brinkman-Rice picture of Mott localisation.

TT 41.9 Wed 11:45 HSZ 204

Quantum Tricritical Points in $NbFe_2$ — •Sven Friedemann[1,2], Max Hirschberger[2,4], Thomas Bauer[3], Robert Kuechler[3], Andreas Neubauer[4], Manuel Brando[3], Christian Pfleiderer[4],

and F Malte Grosche[2] — [1]HH Wills Laboratory, University of Bristol, UK — [2]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Physik Department E21, TU München, Garching, Germany

Quantum critical points (QCPs) in ferromagnetic (FM) metals impose a long-standing challenge including seemingly incompatible temperature dependencies in transport and thermodynamic properties. In many of these systems, the FM QCP is avoided through a change to 1st order. Here, we present results on a second class of FM quantum critical metals in which the QCP is avoided through an intervening spin-density-wave (SDW) phase. We show that the phase diagram of $NbFe_2$ can be modelled with a two-order-parameter theory in which the FM QCP is buried within a SDW phase, as proposed by Moriya and Usami [1]. This model reproduces detailed magnetisation measurements on high-purity single crystals for a series of samples tuned across the buried FM QCP via variations in the composition. We establish the presence of quantum tricritical points at which both the uniform and finite wavelength susceptibility diverge, which may explain the incompatible temperature dependencies.
[1] Sol State Com, **23** 935 (1977)

TT 41.10 Wed 12:00 HSZ 204

Effect of tuning parameters on the partially frustrated magnetic order in CePdAl — •Stefan Lucas[1,2], Zita Hüsges[3], Veronika Fritsch[4], Jens-Uwe Hoffmann[3], Karel Prokeš[3], Manfred Reehuis[3], Hilbert von Löhneysen[5], and Oliver Stockert[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Institute of Solid State Physics, TU Dresden, Dresden, Germany — [3]Helmholtz-Zentrum Berlin, Berlin, Germany — [4]EP 6, Electronic Correlations and Magnetism, Augsburg University, Augsburg, Germany — [5]Karlsruhe Institute of Technology, Institute for Solid State Physics, Karlsruhe, Germany

The heavy-fermion system CePdAl is a model system to investigate magnetic frustration in a metallic material. An arrangement of the Ce moments on a distorted kagomé lattice in the basal plane together with a strong Ising anisotropy leads to geometric frustration. This results in a complex interplay with the RKKY and Kondo interaction, where only two thirds of the magnetic moments are long-range ordered, whereas the remaining third is frustrated and/or screened by the Kondo effect below the antiferromagnetic ordering temperature of 2.7 K. Using different in-plane tuning parameters like magnetic fields and especially uniaxial pressure, we investigated the stability of the complex magnetic order. Thereby, we were able to stabilize the magnetic order under moderate uniaxial pressures of up to 1 kbar.

TT 41.11 Wed 12:15 HSZ 204

Signature of frustrated moments in quantum critical $CePd_{1-x}Ni_xAl$ — Akito Sakai[1], Stefan Lucas[2], Zita Huesges[2], Kai Grube[3], Philipp Gegenwart[1], Oliver Stockert[2], Hilbert v. Löhneysen[3], and •Veronika Fritsch[1] — [1]EP 6, Electronic Correlations and Magnetism, Augsburg University, Germany — [2]Max Planck Insitute for Chemical Physics of Solids, Dresden, Germany — [3]Institute for Solid State Physics and Physics Institute, Karlsruhe Institute of Technology, Germany

Magnetic frustration suppresses long-range magnetic order despite the presence of strong magnetic couplings. This results in exotic ground states, where the spins can fluctuate down to zero temperature. However, metallic materials that simultaneously exhibit magnetic frustration and a strong coupling between the magnetic moments and the conduction electrons, are quite scarce.

The here presented CePdAl is a system were the Kondo effect and magnetic frustration coexist. It can be tuned across a quantum critical point by substitution of Pd with approximately 14% of Ni. Furthermore, field-induced quantum criticality can be observed in $CePd_{1-x}Ni_xAl$. We have investigated single crystals with Ni concentrations $0 \leq x \leq 0.16$. In addition to the generic signatures of quantum criticality a unique thermodynamic feature of the frustrated moments, i.e. an additional contribution to the magnetic Grüneisen paramter, is discovered [1].
[1] A. Sakai *et al.*, ArXiv:1609.00816 [cond-mat.str-el] (2016).

TT 41.12 Wed 12:30 HSZ 204

$YbNi_4(P_{1-x}As_x)_2$: Single crystal growth and characterization — •Kristin Kliemt[1], Philipp Ross[1], Oliver Stockert[2], Manuel Brando[2], and Cornelius Krellner[1] — [1]Goethe-University Frankfurt, Institute of Physics, 60438 Frankfurt, Germany — [2]MPI CPfS, 01187 Dresden, Germany

The low lying Curie temperature, $T_C = 0.17$ K, of the heavy-fermion compound $YbNi_4P_2$ can be further suppressed by substituting P by As and the rare case of a ferromagnetic quantum critical point occurs in the substitution series $YbNi_4(P_{1-x}As_x)_2$ at $x \approx 0.1$ [1,2].

Here, we present the growth of $YbNi_4(P_{1-x}As_x)_2$ single crystals with As concentrations from $0 \leq x \leq 1$ using the Czochralski method from a levitating melt. Recently, this crucible free growth method was successfully implemented to obtain cm-sized oriented single crystals of the unsubstituted compound $YbNi_4P_2$ [3]. The samples were characterized by electrical transport, heat capacity and magnetization measurements and we will give details about these results. Furthermore, we determined their crystal structure by powder X-ray diffraction and investigated the homogeneity of the As distribution in the crystals using energy dispersive X-ray spectroscopy. In addition, the crystallinity of the samples was checked by neutron Laue backscattering.
[1] C. Krellner et al., New J. Phys. 13, 103014 (2011)
[2] A. Steppke et al., Science 339, 933 (2013)
[3] K. Kliemt, C. Krellner, J. Cryst. Growth 449, 129 (2016).

TT 41.13 Wed 12:45 HSZ 204

Magneto-acoustic investigations of field-induced quantum criticality in Cs_2CuCl_4 — •Bernd Wolf[1], Lars Postulka[1], Yeekin Tsui[1], Pham Thang Cong[1,2], Natalia van Well[1,3], Franz Ritter[1], Cornelius Krellner[1], and Michael Lang[1] — [1]Physics Institute, Goethe University Frankfurt, D-60438 Frankfurt(M) — [2]Dresden-HFFL, Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden — [3]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, CH-5232 Villigen

Magnetoelastic investigations of the frustrated triangular-lattice antiferromagnet Cs_2CuCl_4 were performed for the longitudinal modes c_{11}, c_{22} and c_{33} in magnetic fields up to 10 T and down to 0.032 K. Acoustic anomalies have been found both in the temperature and in the field dependence of these modes. For temperatures $0.8\ \mathrm{K} > T > 2.0$ K in the 1D-regime of Cs_2CuCl_4, the magnetoelastic behaviour can be well described with a microscopic theory. The field-dependent measurements for $T > T_N$ around the quantum-critical point (QCP) at $B_s \sim 8.5$ T display two distinct anomalies which are attributed to the transition into long-range afm order and signatures of the preceding spin-liquid state. At the lowest temperatures of our experiment $c_{33}(B)$ can be well described by a Landau free energy model with a very small magnetoelastic coupling constant $G/k_B = 2.8$ K. The observation of rather classical behaviour at lowest temperatures and the deviations from the classical behaviour at somewhat higher temperatures are assigned to the opening of a small gap in the magnetic excitations spectrum for $B < B_s$ which drives the system away from quantum criticality.

TT 42: Correlated Electrons: Frustrated Magnets - Strong Spin-Orbit Coupling 2

Time: Wednesday 9:30–13:00 Location: HSZ 304

TT 42.1 Wed 9:30 HSZ 304

Thermal transport in Kitaev spin systems — •Wolfram Brenig and Alexandros Metavitsiadis — Institute for Theoretical Physics, Technical University Braunschweig, Germany

We study the dynamical thermal conductivity of Kitaev spin models on two-leg ladders and honeycomb lattices. In contrast to the majority of conventional one-dimensional spin systems, we show the ladder to represent the rare case of a perfect heat insulator. This is a direct consequence of fractionalization of spins into mobile Majorana matter and static Z_2 gauge fields. Our findings rest on complementary calculations of the current correlation function, comprising a mean-field treatment of thermal gauge fluctuations, a complete summation over all gauge sectors, as well as exact diagonalization of the original spin model. On the honeycomb lattice results will be presented from high temperature numerical diagonalization and from low temperature perturbation theory.

TT 42.2 Wed 9:45 HSZ 304

Three-band Hubbard model for Na_2IrO_3: Topological insulator, zigzag antiferromagnet, and Kitaev-Heisenberg material — •Stephan Rachel[1], Manuel Laubach[1], Ronny Thomale[2], and Johannes Reuther[3] — [1]TU Dresden, Institut für Theoretische Physik — [2]Universität Würzburg, Institut für Theoretische Physik — [3]FU Berlin & Helmholtz-Zentrum Berlin

Na_2IrO_3 was one of the first materials proposed to feature the Kane-Mele type topological insulator phase. About the same time it was claimed that the very same material is in a Mott insulating phase which is described by the Kitaev-Heisenberg (KH) model. First experiments indeed revealed Mott insulating behavior in conjunction with antiferromagnetic long-range order. Further refined experiments established antiferromagnetic order of zigzag type which is not captured by the KH model. Since then several extensions and modifications of the KH model were proposed in order to describe the experimental findings. Here we suggest that adding charge fluctuations to the KH model represents an alternative explanation of zigzag antiferromagnetism. Moreover, a phenomenological three-band Hubbard model unifies all the pieces of the puzzle: topological insulator physics for weak and KH model for strong electron-electron interactions. And at moderate interaction strength we find a zigzag antiferromagnet.

TT 42.3 Wed 10:00 HSZ 304

Honeycomb-lattice Heisenberg-Kitaev model in a magnetic field: Spin canting, metamagnetism, and vortex crystals — •Lukas Janssen[1], Eric C. Andrade[2], and Matthias Vojta[1] — [1]Technische Universität Dresden, Germany — [2]Universidade de São Paulo, Brazil

The Heisenberg-Kitaev model is a paradigmatic model to describe the magnetism in honeycomb-lattice Mott insulators with strong spin-orbit coupling, such as A_2IrO_3 (A = Na, Li) and α-$RuCl_3$. In this talk, I present in detail the physics of the Heisenberg-Kitaev model in an external magnetic field. Using the combined results of Monte-Carlo simulations and spin-wave theory the classical phase diagram for different directions of the magnetic field is mapped out. Broken SU(2) spin symmetry renders the magnetization process rather complex, with sequences of phases and metamagnetic transitions. In particular, various large-unit-cell and multi-Q phases including a vortex-crystal phase occur for a field in the [111] direction. I also discuss quantum corrections in the high-field phase.

[1] L. Janssen, E. C. Andrade, and M. Vojta, arXiv:1607.04640 [cond-mat.str-el] (PRL accepted).

TT 42.4 Wed 10:15 HSZ 304

Spectroscopic investigations of a novel Iridate - a possible reference material for Kitaev physics — Philipp Benrath[1], Angela Möller[1], Vladimir Gnezdilov[2,3], and •Peter Lemmens[2] — [1]IAC-AC, JGU Mainz — [2]TU-BS, Braunschweig — [3]ILTP, Kharvov

In $Na_2Ir(OH)_6$ there exist a D3d point group symmetry with an uniaxial threefold symmetry of the iridium complex. In our search for nonabelian anyons (fractionalized excitations)[1] we performed a systematic Raman scattering investigation of its excitation spectrum. Evidence for a symmetry reduction and its relation to other distorted Kitaev materials are discussed.

Work supported by RTG-DFG 1952/1, the Laboratory for Emerging Nanometrology, TU Braunschweig, and NTH Contacs in Nanosystems.
[1] A. Glamazda, P. Lemmens, S.-H. Do, K.-Y. Choi, Nature Commun. 7, 12286 (2016).

TT 42.5 Wed 10:30 HSZ 304

Electronic structure of α-$RuCl_3$ from electron spectroscopy — •Andreas Koitzsch[1], Carsten Habenicht[1], Eric Müller[1], Martin Knupfer[1], Bernd Büchner[1,2], Hem Kandpal[1,3], Jeroen van den Brink[1,4], Domenic Nowak[5], Anna Isaeva[5], and Thomas Doert[5] — [1]IFW Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, Germany — [3]Indian Institute of Technology, Roorkee, India — [4]Institute for Theoretical Physics, TU Dresden, Germany — [5]Department of Chemistry and Food Chemistry, TU Dresden, Germany

Novel ground states might be realized in honeycomb lattices with strong spin–orbit coupling. Here we study the electronic structure of α-$RuCl_3$, in which the Ru ions are in a d^5 configuration and form a honeycomb lattice, by angle-resolved photoemission, x-ray photoemission and electron energy loss spectroscopy supported by density functional theory and multiplet calculations. We find that α-$RuCl_3$ is a Mott insulator with significant spin-orbit coupling, whose low energy electronic structure is naturally mapped onto J_{eff} states. This makes α-$RuCl_3$ a promising candidate for the realization of Kitaev physics. Relevant electronic parameters such as the Hubbard energy U, the crystal field splitting $10Dq$ and the charge transfer energy Δ are evaluated.

TT 42.6 Wed 10:45 HSZ 304

Field-induced changes of the thermodynamic properties of the honeycomb system α-$RuCl_3$ — •A.U.B. Wolter[1], L.T. Corredor[1], M. Geyer[1], K. Nenkov[1], R. Hühne[1], S.-H. Do[3], K.-Y. Choi[3], Y.S. Kwon[4], A. Isaeva[5], D. Nowak[5], T. Doert[5], L. Janssen[6], M. Vojta[6], and B. Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01062 Dresden, Germany — [3]Department of Physics, Chung-Ang University, Seoul 156-756, Republic of Korea — [4]Department of Emerging Materials Science, DGIST, Daegu 711-873, Republic of Korea — [5]Department of Chemistry and Food Chemistry, TU Dresden, 01062 Dresden, Germany — [6]Institute for Theoretical Physics, TU Dresden, 01062 Dresden, Germany

α-$RuCl_3$ with its honeycomb lattice and strong spin-orbit coupling has been at the center of attention in the last two years, since it has been proposed as a prime candidate to study fractionalized Kitaev physics despite its zigzag antiferromagnetic ground state. The thermal fractionalization of quantum spins in a Kitaev model has been predicted to be experimentally observable in e.g. the specific heat, and transport properties. We studied the thermodynamic behavior of this system by means of a detailed specific heat investigation in applied magnetic fields up to 14 T. Our studies reveal an angular dependent suppression of the long-range magnetic order in applied magnetic fields, as well as a pronounced suppression of the specific heat at low temperatures and high fields, suggesting the appearance of a gapped state. This scenario is discussed in light of a detailed entropy analysis in both regimes.

TT 42.7 Wed 11:00 HSZ 304

Anisotropic Ru^{3+} magnetism in the honeycomb system α-$RuCl_3$ — •Maximilian Geyer[1,2], Laura Theresa Corredor Bohorquez[1], Sebastian Gass[1], Synho Do[3], Kwangyong Choi[3], Yong Seung Kwon[3], Anna Isaeva[4], Domenic Nowak[4], Thomas Doert[4], Anja U.B. Anja U.B. Wolter[1], and Bernd Büchner[1,2] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01062 Dresden, Germany — [3]Department of Physics, Chung-Ang University, Seoul 156-756, Republic of Korea — [4]Department of Chemistry and Food Chemistry, TU Dresden, 01062 Dresden, Germany

The interplay between electronic correlations and spin-orbit coupling in heavy transition metal compounds has been intensively studied in the last years due to their interesting properties and unusual ground states like quantum spin liquids. Particularly, α-$RuCl_3$ shows interest-

ing properties, which can be attributed to its proximity to a Kitaev spin liquid state. We report on magnetization measurements for α-$RuCl_3$ single crystals grown by means of chemical vapor transport reactions. The main focus lies on angular dependent measurements and the behavior of α-$RuCl_3$ in high magnetic fields in order to understand the highly anisotropic magnetism in this layered compound.

15 min. break.

TT 42.8 Wed 11:30 HSZ 304

Transport studies of the Kitaev-Heisenberg compound α-$RuCl_3$ — •Richard Hentrich[1,2], Bernd Büchner[1,2], Domenic Nowak[3], Anna Isaeva[3], Thomas Doert[3], Jennifer Sears[4], Young-June Kim[4], Paula J. Kelley[5], Stephen E. Nagler[5], and Christian Hess[1,2] — [1]IFW Dresden, Germany — [2]Center for Transport and Devices of Emergent Materials, TU Dresden, Germany — [3]Inorganic Chemistry Department II, TU Dresden, Germany — [4]Department of Physics, University of Toronto, Canada — [5]Oak Ridge National Laboratory, USA

α-$RuCl_3$ is a material composed of weakly van der Waals bound honeycomb layers of edge sharing $RuCl_6$ octahedra with the central atom being in a $J_{\text{eff}} = 1/2$ state. This kind of strongly frustrated spin structure is a candidate for Kitaev-Heisenberg physics which features non-trivial, fractionalised excitations.
Thermal transport measurements are known as a valuable tool to probe elementary excitations of systems with low dimensional spin structure and are possibly suited to detect Majorana fermionic contributions to the net heat conductivity.
We observe strong suppression of the phononic in-plane thermal conductivity of α-$RuCl_3$ single crystals at low temperatures in zero magnetic field. However, upon applying an external magnetic field the heat conductivity is strongly enhanced. We interpret our findings in terms of a field-induced quantum phase transition.

TT 42.9 Wed 11:45 HSZ 304

Single, double, and triple spin-orbit excitons in α-$RuCl_3$ — •Nick Borgwardt[1], Alessandro Revelli[1], Maria Hermann[2], Petra Becker[3], Paul van Loosdrecht[1], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für theoretische Physik, Universität zu Köln — [3]Abteilung Kristallographie, Institut für Geologie und Mineralogie, Universität zu Köln

Spin-orbit-assisted d^5 Mott insulators with local j=1/2 moments are discussed as realizations of the Kitaev model which hosts Majorana fermion excitations. In promising candidate materials such as $RuCl_3$, lattice distortions give rise to a mixing of j=1/2 and 3/2 character which may spoil the picture. The so-called spin-orbit exciton corresponds to an excitation to the j=3/2 state and is very sensitive to the character of the relevant states. In the literature, features in Raman scattering, neutron scattering, and infrared absorption data were reported in the relevant frequency range of one to a few hundred meV. We challenge the reported interpretations and demonstrate that our infrared data show single, double, and triple spin-orbit excitons. These novel and unusual excitations are directly connected to the microscopic processes relevant for the Kitaev coupling.

TT 42.10 Wed 12:00 HSZ 304

Raman Spectroscopy on the putative Kitaev Material $RuCl_3$ — •Thomas Koethe[1], Sebastian Kaul[1], Raphael German[1], Petra Becker[2], Markus Grüninger[1], and Paul van Loosdrecht[1] — [1]Institute of Physics 2, University of Cologne — [2]Institute for Geology and Mineralogy, University of Cologne

The famous Kitaev model with bond-directional Ising-type interactions on tricoordinated lattices allows for an exotic spin liquid ground state and Majorana fermion excitations. Real materials like the spin-orbit driven Mott insulator $RuCl_3$ usually show an additional isotropic Heisenberg interaction competing with the Kitaev interactions. Raman spectroscopy is an excellent tool to investigate unconventional states of matter and provides information not only about the electronic ground state of the material, whose $j = 1/2$ nature is a requirement for the Kitaev physics, but also about the nature of the excitations. Though we observe a low energy scattering continuum, our results do not seem to be compatible with current theoretical predictions for the Majorana continuum. We do see, however, a Fano-type phonon continuum coupling which may be compatible with theoretical expectations. Electronic excitations at higher energies challenge the previously proposed electronic structure of the material.

TT 42.11 Wed 12:15 HSZ 304

Effect of symmetry and local distortions on fractionalized excitations in Kitaev Systems — •Peter Lemmens[1], Vladimir Gnezdilov[1,2], Alexander Glamazda[1,2,3], S.-H. Do[3], K.-Y. Choi[3], Angela Möller[4], Friedrich Freund[5], and Philipp Gegenwart[5] — [1]TU-BS Braunschweig — [2]ILTP Kharkov — [3]CAU Seoul — [4]IAC-AC, JGU Mainz — [5]EP-VI, ZEKM, Augsburg

In Kitaev physics the role of symmetry is crucial. A prerequisite of the Kitaev model demands uniaxial threefold symmetry of the iridium complex. [1,2] Therefore, the comparison of different systems representing the Kitatev model on different honeycomb-like lattices [3] is an important topic. We performed Raman scattering investigations on the continuum of fractionalized excitations to understand the role of symmetry, local distortions and dimensionality. In detail, we will report on data of α-$RuCl_3$ as well as 2D/3D $(Na,Li)_2IrO_3$ and related compounds.

Work supported by RTG-DFG 1952/1, the Laboratory for Emerging Nanometrology, TU Braunschweig, and NTH Contacs in Nanosystems.
[1] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. 102, 017205 (2009)
[2] M. Becker, M. Hermanns, B. Bauer, M. Garst and S. Trebst, Phys. Rev. B 91, 155135 (2015)
[3] A. Glamazda, P. Lemmens, S.-H. Do, K.-Y. Choi, Nature Commun. 7, 12286 (2016).

TT 42.12 Wed 12:30 HSZ 304

Disorder and topology in a periodically driven Kitaev model — •Mykola Maksymenko[1,2], Maria-Theresa Rieder[2], Ion Cosma Fulga[2], Netanel Lindner[3], and Erez Berg[2] — [1]Institute for Condensed Matter Physics of NAS of Ukraine, Lviv-79011, Ukraine — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, 76100, Israel — [3]Physics Department, Technion, 320003 Haifa, Israel

We investigate a periodically driven 2D Kitaev model in which anisotropic exchange integrals are boosted at consecutive time intervals. This model shows a rich phase diagram consisting of novel anomalous topological phases. Unlike the static Kitaev model some of the phases, can host pairs of Majorana modes at a single vortex defect or lattice dislocation. We characterize the different phases using weak and strong scattering-matrix invariants defined for the corresponding fermionic model and investigate their stability to different types of disorder.

TT 42.13 Wed 12:45 HSZ 304

Topological Superconductivity in the Extended Kitaev-Heisenberg Model — •Johann Schmidt, Tomas Löthman, and Annica M. Black-Schaffer — Uppsala Universitet, Uppsala, Schweden

We extend the discussion of superconductivity in the Kitaev-Heisenberg model by taking into account the recently proposed symmetric off-diagonal exchange term Γ. The new interaction term contributes further to the triplet superconductivity triggered by the Kitaev exchange. While a positive Γ bolsters the already reported time-reversal symmetric p-wave state with its transition to a topologically non-trivial state at high doping levels, new superconducting orders emerge for negative values of Γ. Of particular interest is a region at intermediate doping which breaks time-reversal symmetry and can be classified by a Chern number of ± 2.

TT 43: Two-Dimensional Materials IV (joint session DS, HL, TT, organized by HL)

Time: Wednesday 9:30–13:15 Location: POT 51

TT 43.1 Wed 9:30 POT 51

Landau-Quantized Graphene: A Tunable Nonlinear Optical Material in the THz Range — •Jacob C. König-Otto[1,2], Yongrui Wang[3], Alexey Belyanin[3], Claire Berger[4,5], Walt A. de Heer[4], Milan Orlita[6,7], Alexej Pashkin[1], Harald Schneider[1], Manfred Helm[1,2], and Stephan Winnerl[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Technische Universität Dresden, Germany — [3]Texas AM University, USA — [4]Georgia Institute of Technology, USA — [5]CNRS-Université Alpes, France — [6]LNCMI, Grenoble, France — [7]Charles University in Prague, Czech Republic

Finding nonlinear optical materials for the THz and mid-infrared regimes is not straightforward. State-of-the-art devices with a high third-order optical susceptibility are often processed as complex multi-quantum-well structures designed to feature one specific resonance frequency. In our work we study Landau-quantized graphene as a tunable and simple to produce nonlinear material. To this end we perform time-integrated degenerate four-wave mixing (FWM) experiments at a photon energy of 78 meV resonant to the transitions between the Landau levels LL_{-1}, LL_0 and LL_1 at a magnetic field of roughly 4 T. We can recover expected scaling of the FWM-signal with the incident fields and the resonance behavior. The value of the third-order surface susceptibility in this material is in agreement with our calculations based on the density matrix formalism. We find the order of $\chi^{(3)}$ of Landau-quantized graphene to be competitive with more complex and elaborated solutions.

TT 43.2 Wed 9:45 POT 51

Ballistic transport in 2D periodically modulated graphene — •Andreas Sandner[1], Martin Drienovsky[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]NIMS, 1-1 Namiki, Tsukuba, Japan

Embedding graphene into a heterostructure with hexagonal boron nitride was shown to be an efficient way of achieving a high bulk mobility. The encapsulated graphene is protected in any further top-down fabrication procedure and pronounced commensurability features could be observed in 2D antidot lattices [1].

Here, we want to introduce a new method for periodical modulation of the carrier density, employing a few layer graphene patterned bottom gate. The bottom gate is defined by etching a 2D hole array into the few layer graphene and adapts perfectly to the commonly used stacking method for van der Waals heterostructures. By tuning the local bottom gate and the global back gate voltage, we can switch between the unipolar and bipolar transport regime.

We fabricated patterned bottom gates with lattice periods down to 150 nm and observe pronounced commensurability peaks that can be nicely compared to experiments with hard-wall graphene antidot lattices. We report on the difference between the unipolar and the bipolar regime, as well as the influence of the magnitude of the imposed superlattice potential.

[1] A. Sandner et al., Nano Lett. **15**, 8402 (2015)

TT 43.3 Wed 10:00 POT 51

Commensurability oscillations in electrostatically modulated graphene — •Martin Drienovsky[1], Jonas Joachimsmeyer[1], Takashi Taniguchi[3], Kenji Watanabe[3], Ming-Hao Liu[2], Klaus Richter[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Institut für Theoretische Physik, Universität Regensburg, Germany — [3]National Institute for Material Science, Tsukuba, Japan

We report on the first experimental observation of commensurability oscillations (COs) [1] in a 1D periodic graphene superlattice. Employing a locally acting few layer graphene patterned bottom gate (FLG PBG) and a dry van-der-Waals stacking method we prepare high mobility graphene-boron nitride heterostructures, where the ballistic length exceeds several periods of the modulation. The potential landscape can be tuned by the striped FLG PBG and a global back gate in such a way that a small, periodic and unipolar potential perturbation is generated. The magnetoresistance exhibits well pronounced COs at predicted magnetic field positions for electrostatic modulation, both for the electron and hole transport regime. Our measurements confirm strong robustness of the COs in graphene with respect to temperature [2], as they remain visible up to 155 K.

[1] D. Weiss et al., Europhys. Lett. 8, 179 (1989) [2] A. Matulis and F. M. Peeters, Phys. Rev. B 75, 125429 (2007)

TT 43.4 Wed 10:15 POT 51

Intrinsic mobility due to electron-phonon interaction in black phosphorus. — •Sergey Brener, Alexander Rudenko, and Mikhail Katsnelson — Radboud Universiteit, Niederlanden

Flexural and in-plane thermal fluctuations in crystalline membranes affect the band structure of the carriers, which has an effect on transport properties of 2D systems. I consider a specific example of one-layer black phosphorus, which is a highly anisotropic material, and present our recent results on intrinsic carrier mobility. In contrast to graphene, where the mobility is determined by two-phonon (flexural) scattering, in black phosphorus one-phonon (in-plane) processes dominate.

TT 43.5 Wed 10:30 POT 51

Strain-induced commensurability oscillations in graphene — •Jonas Joachimsmeyer[1], Martin Drienovsky[1], Takashi Taniguchi[2], Kenji Watanabe[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

We realized a periodic strain modulation in a graphene/hexagonal boron-nitride (hBN) heterostructure by transferring it onto a prepatterned 1D superlattice etched into hBN. The transfer was performed using a dry van-der-Waals pick-up technique. This method yields a high mobility graphene device with a mean free path exceeding the period of the corrugation.

We conducted magnetotransport experiments in this corrugated graphene monolayer with a period of 150 nm. The modulation leads to a periodic strain which in turn gives rise to an effective periodic pseudopotential with half of the period of the corrugation [1], i.e. 75 nm. Due to the periodic potential we observe commensurability oscillations (COs) [2] in the longitudinal magnetoresistance, however superimposed by Shubnikov-de Haas (SdH) oscillations. Since both oscillations show different temperature dependences we increased the temperature up to 80 K. While the SdH oscillations get suppressed the COs still remain visible.

[1] Burgos, R., and Lewenkopf, C., arXiv:1610.04068 (preprint 2016).
[2] Ye, P. D., Weiss, D., et al., Semicond. Sci. Technol. 10, 715 (1995).

TT 43.6 Wed 10:45 POT 51

Temperature switchable type of conductivity in hybrid conjugated polyelectrolyte/graphene two-dimensional nanocomposites — •Viktor Brus[1], Marc Gluba[1], Cheng-Kang Mai[2], Stefany Fronk[2], Jörg Rappich[1], Norbert Nickel[1], and Cuillermo Bazan[2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekuléstr. 5, 12489 Berlin, Germany — [2]Center for Polymers and Organic Solids, Department of Chemistry and Biochemistry, University of California at Santa Barbara, Santa Barbara, CA, 93106, USA

We found that a submonolayer of CPE-PyrBIm4 on CVD-grown graphene forms a novel two-dimensional hybrid material that exhibits preferential transport of holes or electrons as a function of temperature. Doping efficiencies increase with the increase of the temperature used to anneal the heterobilayers and a decrease of the CPE-PyrBIm4 film thickness. The switching of the conductivity type of the thin CPE-PyrBIm4/graphene heterobilayer composite occurs when graphene is not strongly overcompensated. Moreover, the conversion of the conductivity type is reversible. Doping mechanisms under consideration include charge transfer from electron rich structural units in the CPE-PyrBIm4 backbone and/or field-effect doping as a result of interfacial electrostatic effects from adjacent ionic functionalities. This effect shows the unique and complex nature of electrical properties of the novel heterobilayer hybrid organic-inorganic CPE-PyrBIm4/graphene nanocomposite material and enhances interest in further investigations.

TT 43.7 Wed 11:00 POT 51

Interlayer screening in n-doped bilayer and trilayer transition metal dichalcogenides — •Andor Kormányos[1], Viktor Zólyomi[2], and Guido Burkard[1] — [1]University of Konstanz, Germany — [2]Manchester University, United Kingdom

We derive an effective Hamiltonian based on the k.p approach that describes the dispersion at the band edges of the conduction band of bilayer and trilayer transition metal dichalcogenides (TMDCs). This model is then used to consider n-doped bilayer MoS_2 placed in uniform external electric field. We discuss the charge re-distribution between the layers due to the electric field and calculate the bandgap that opens at the K-point of the Brillouin zone in self-consistent Hartree approximation. We point out the relation between the induced band-gap and the quantum capacitance and briefly discuss the relevance of our results to recent photoluminiscence experiments in double gated bilayer MoS_2.

Coffee Break

TT 43.8 Wed 11:45 POT 51

Driven Hofstadter Butterflies — •Martin Wackerl[1] and John Schliemann[2] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Institut für Theoretische Physik, Universität Regensburg

Periodically driven quantum systems offer a great way of tuning band structures or Chern numbers. The first part will be about graphene illuminated with circular polarized light. The external driving is introduced via the Floquet formalism and the main focus will be on the deformation of the band structure of graphene. Afterwards we will give a short introduction to the Hofstadter butterfly and unify it with the Floquet formalism. We will show how the Hofstadter spectrum gets distorted when tuning the light intensity, photon energy, and polarization. The last part is about the influence of polarized light to the distribution of ground state Chern numbers of the Floquet-Hofstadter spectrum.

TT 43.9 Wed 12:00 POT 51

Resonant scattering off adatoms in monolayer graphene — •Susanne Irmer, Denis Kochan, and Jaroslav Fabian — University of Regensburg, Regensburg, Germany

We present a theoretical investigation of resonant scattering off adatoms on graphene. Resonant scattering is an important feature of adatoms as it leads to resonant enhancement of the impact of proximity effects such as local magnetic moments or spin-orbit coupling [1,2,3]. We investigate the three different adsorption positions of hollow, top, and bridge employing effective realistic tight-binding models and the T-matrix formalism. The developed resonance conditions are useful for quantum transport models as well as studies of spin relaxation in graphene with adatoms.

This work was supported by the DFG SFB 689 and GRK 1570, and by the European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

[1] D. Kochan, M. Gmitra, and J. Fabian, Phys. Rev. Lett. 112, 116602 (2014)

[2] J. Bundesmann, D. Kochan, F. Tkatschenko, J. Fabian, and K. Richter, Phys. Rev. B 92, 081403 (2015)

[3] D. Kochan, S. Irmer, and J. Fabian, arXiv:1610.08794

TT 43.10 Wed 12:15 POT 51

Experimental realization and characterization of an electronic Lieb lattice — •Marlou Slot[1], Thomas Gardenier[1], Peter Jacobse[1], Guido van Miert[2], Sander Kempkes[2], Stephan Zevenhuizen[1], Cristiane Morais Smith[2], Daniel Vanmaekelbergh[1], and Ingmar Swart[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, Netherlands — [2]Institute for Theoretical Physics, Utrecht University, Netherlands

Geometry, whether on the atomic or nanoscale, is a key factor for the electronic band structure of materials. For example, the honeycomb geometry leads to Dirac-type bands where the charge carriers behave as massless particles. Theoretical predictions are triggering the exploration of novel 2D geometries, such as graphynes, Kagomé and the Lieb lattice. The latter is the 2D analogue of the 3D lattice exhibited by perovskites; it is a square-depleted lattice, which is characterised by a band structure featuring Dirac cones intersected by a topological flat band. Whereas photonic and cold-atom Lieb lattices have been demonstrated, an electronic equivalent in 2D is difficult to realize in an existing material. Here, we report an electronic Lieb lattice formed by the surface state electrons of Cu(111) confined by an array of CO molecules positioned with a scanning tunneling microscope. Using scanning tunneling spectroscopy and wave-function mapping, we confirm the characteristic electronic structure of the Lieb lattice. The experimental findings are corroborated by muffin-tin and tight-binding calculations. At higher energy, second-order electronic patterns are observed, which are equivalent to a super-Lieb lattice.

TT 43.11 Wed 12:30 POT 51

Interlayer Configuration in Twisted Bilayers of Folded Graphene — •Johannes C. Rode, Christopher Belke, Hennrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

Twisted bilayer graphene (TBG), i.e. stacks of two graphene sheets in arbitrary rotational misalignment, exhibit rich electronic spectra[1,2] which are highly dependent on the interlayer twist angle in general[3] as well as details in stacking configuration like lattice commensuration and corrugation[4] in particular. We here examine the latter TBG properties coming from the morphological side: TBG are prepared via Atomic Force Microscope, folding ribbons out of monolayer sheets. In the recently proposed picture of a thermally activated growth process[5], here measured quantities like interlayer distance and shape of the folded edge are found to hold novel information about angle-dependent interlayer configuration and provide insight about interaction in van der Waals bound materials.

[1] H. Schmidt; J. C. Rode; D. Smirnov; R. J. Haug, Nat. Comm. **5**, 5742 (2014).

[2] J. C. Rode; D. Smirnov; H. Schmidt, R. J. Haug, 2D Materials **3**, 035005 (2016).

[3] J. M. B. Lopes dos Santos; N. M. R. Perez; A. H. Castro Neto, Phys. Rev. Lett. **99**, 25682 (2007).

[4] E. J. Mele, Phys. Rev. B **81**, 161405(R) (2010).

[5] J. Annett; G. L. W. Cross, Nature **535**, 271-275 (2016).

TT 43.12 Wed 12:45 POT 51

Multi-scale approach for strain-engineering of phosphorene — Daniel Midtvedt[1] and •Alexander Croy[2] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany

A multi-scale approach for the theoretical description of deformed phosphorene is presented. This approach combines a recently developed valence-force model [1] to relate macroscopic strain to microscopic displacements of atoms and a tight-binding model [2] with distance-dependent hopping parameters to obtain electronic properties. The resulting self-consistent electromechanical model is suitable for large-scale modeling of phosphorene devices. We demonstrate this for the case of an inhomogeneously deformed phosphorene drum, which may be used as an exciton funnel [3].

[1] D. Midtvedt and A. Croy, Phys. Chem. Chem. Phys. 18, 23312 (2016). [2] A. N. Rudenko, S. Yuan, and M. I. Katsnelson, Phys. Rev. B 92, 085419 (2015). [3] P. San-Jose et al, Phys. Rev. X 6, 031046 (2016).

TT 43.13 Wed 13:00 POT 51

Evolution of electronic structure of few-layer phosphorene from angle-resolved photoemission spectroscopy of black phosphorous — •Niels Ehlen[1], Boris Senkovskiy[1], Alexander Fedorov[1,2,3], Andrea Perucchi[4], Paola Di Pietro[4], Antonio Sanna[5], Gianni Profeta[6], Luca Petaccia[4], and Alexander Grüneis[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]IFW Dresden, Germany — [3]St. Petersburg State University, Russia — [4]Elettra Sincrotrone Trieste, Italy — [5]Max Planck Institute of Microstructure Physics, Halle, Germany — [6]Department of Physical and Chemical Sciences/SPIN-CNR, University of L'Aquila, Italy

A complete set of tight-binding parameters for the description of the quasiparticle dispersion relations of black phosphorous (BP) and N-layer phosphorene with $N = 1 \ldots \infty$ is presented. The parameters, which describe valence and conduction bands, are fit to angle-resolved photoemission spectrocopy (ARPES) data of pristine and lithium doped BP. We show that zone-folding of the experimental three-dimensional electronic band structure of BP is a simple and intuitive method to obtain the layer-dependent two-dimensional electronic structure of few-layer phosphorene. Zone-folding yields the band gap of N-layer phosphorene in excellent quantitative agreement to experiments and *ab-initio* calculations. A combined analysis of optical absorption and ARPES spectra of pristine and doped BP are used to estimate a value for the exciton binding energy of BP.

TT 44: Focus Session: Non-Equilibrium Dynamics in Light-Driven Materials: Theory Meets Experiment (joint session O, TT, organized by O)

Time: Wednesday 10:30–13:00 Location: TRE Phy

Invited Talk TT 44.1 Wed 10:30 TRE Phy
Electronic orders in light-driven materials — •Philipp Werner[1], Yuta Murakami[1], Hugo Strand[1], Shintaro Hoshino[2], and Martin Eckstein[3] — [1]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — [2]RIKEN Center for Emergent Matter Science, Wako, 351-0198 Saitama, Japan — [3]Max Planck Research Department for Structural Dynamics, University of Hamburg-CFEL, 22761 Hamburg, Germany

The prospect of nonequilibrium control of material properties has caught the interest of the condensed matter community. In particular, recent experiments demonstrating a light-enhanced superconducting-like state in cuprates and fulleride compounds has triggered a number of theoretical studies on order parameter dynamics in lattice systems perturbed by periodic driving or strong quasi-static fields.

Here, we use the nonequilibrium dynamical mean field theory in a Kadanoff-Baym and Floquet implementation to address some relevant issues which have been ignored in previous studies. In particular, we will consider parametric phonon driving in the Holstein model, and show that the nonthermal energy distribution in the driven state generically leads to a weakening of the superconducting order.

As a second example, we will discuss order parameter switching by quasi-static electric fields in fulleride compounds. Here, we will focus on the Jahn-Teller metal phase, which has recently been identified as an orbital-selective Mott state. Electric field pulses can switch this composite ordered state between physically distinct realizations, which may be potentially exploited in ultrafast persistent memory devices.

Invited Talk TT 44.2 Wed 11:00 TRE Phy
Pump/probe photoemission spectroscopy in charge density wave insulators — •James Freericks — Department of Physics, Georgetown University, Washington, DC 20057

In this talk, I will discuss time-resolved photoemission spectroscopy in charge-density-wave (CDW) insulators that form due to an electronic nesting instability. A strongly correlated electronic CDW has a number of interesting features. As the temperature is raised, the gap in the spectrum remains unchanged all the way up to Tc, while the gap fills with subgap states, which eventually metallize the system. There is a critical interaction strength where the metallization occurs the instant the temperature is increased from 0. The system also displays Mott-like physics at strong interaction strength. We illustrate that these systems have an interesting response to the pump. In some cases, the gap region fills in due to the pump, implying the disappearance of the spectral gap, but in the presence of a well formed spatial charge-density-wave order parameter. At the critical interaction strength, the system is exceedingly difficult to pump. Whatever energy is pumped in on the leading edge of the electric field, is pumped out on the trailing edge. These calculations result from the exact solution of the nonequilibrium Falicov-Kimball model via dynamical mean-field theory. We also discuss experimental implications for these results.

Invited Talk TT 44.3 Wed 11:30 TRE Phy
Controlling magnetism and pairing in a periodically driven Hubbard model — •Stephen Clark[1,2], Jonathan Coulthard[3], Juan Jose Mendoza-Arenas[4], Martin Eckstein[2], Dieter Jaksch[3], and Andrea Cavalleri[2,3] — [1]Department of Physics, University of Bath, UK — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [3]Department of Physics, University of Oxford, UK — [4]Departamento de Fisica, Universidad de los Andes, Colombia

In this talk I will describe theory work illustrating striking effects of periodic driving for three different regimes: (i) high frequency $\omega \gg U, t$, (ii) resonant $\omega = nU$ and (iii) in-gap $U \gg \omega \gg t$. Floquet theory when $U \gg t$ predicts renormalisation of t for (i), substantial modifications of both t and U for (ii) and a suppression of t with super-exchange J essentially unchanged for (iii). To demonstrate this physics I will outline non-equilibrium DMFT results showing how the mechanism governing the magnetic melting of an initial classical Neel state can be controlled and switched in the half-filled Hubbard model in infinite dimensions. I will also describe how attaining dominant super-exchange interactions in regime (iii) leads to the emergence of strong singlet-pairing correlations in the driven state. This is demonstrated in the one-dimensional Hubbard model below half-filling in the thermodynamic limit using time-dependent DMRG calculations. By spanning different fillings, dimensions and driving regimes these results show how periodic driving leads to compelling new pathways for controlling magnetism and potentially engineering light-induced superconductivity.

Invited Talk TT 44.4 Wed 12:00 TRE Phy
Ultrafast Terahertz and XUV ARPES Probes of Quantum Materials Dynamics — •Robert A. Kaindl — Materials Sciences Division, E. O. Lawrence Berkeley National Laboratory, Berkeley, USA

In this talk I will discuss the application of ultrashort light pulses - from THz to Extreme-UV - to the study of vibrational coupling and emergent correlations in quantum materials. Transition-metal oxides, in particular, exhibit an intriguing self-organization of charges into nanoscale "stripes", whose driving forces and role in high-Tc superconductivity remain unresolved. We will first present transient multi-THz and mid-IR experiments that capture the initial steps of vibrational symmetry breaking and charge ordering in stripe-phase nickelates, indicating the precursor role of charge localization and exposing the electronic and structural coupling dynamics [1]. In the second part, I will discuss our development of ultrafast angle-resolved photoemission spectroscopy (ARPES) with extreme-ultraviolet (XUV) pulses at 50-kHz repetition rate, and its application to sensitively access electronic dynamics of quantum materials across momentum space [2]. Studies of semiconducting and correlated dichalcogenides access the crossover of light-induced perturbation and melting of charge density waves and provide evidence for excitonic signatures in ARPES spectra. [1] G. Coslovich, et al. Nature Comm. 4, 2643 (2013); arXiv:1603.07819 (2016). [2] H. Wang, et al. Nature Comm. 6, 7459 (2015); J. H. Buss, et al. in preparation (2016).

Invited Talk TT 44.5 Wed 12:30 TRE Phy
Ultrafast spin interactions revealed with terahertz radiation — •Tobias Kampfrath — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The terahertz (THz) frequency range is attracting increasing interest for both applied and fundamental reasons. First, bit rates in current information technology may soon approach the THz range. Second, its low photon energy (4.1 meV at 1 THz) makes THz radiation an excellent probe and stimulus of many fundamental excitations of solids, for instance phonons and Cooper pairs. This talk considers experiments showing that THz pulses are also a very useful and versatile tool to reveal spin interactions on the time scales of elementary relaxation processes. Examples include (i) the ultrafast transfer of energy and angular momentum between phonons and the ordered electron spins of the textbook ferrimagnet yttrium iron garnet (YIG) as well as (ii) the femtosecond transport of magnons across the interface of the spin Seebeck bilayer system YIG/Pt.

TT 45: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - IV (joint session DS, HL, MA, MM, O, TT, organized by O)

Time: Wednesday 10:30–13:00 Location: GER 38

Invited Talk TT 45.1 Wed 10:30 GER 38

Electronic excitations in 2D materials and heterostructures — •Kristian Sommer Thygesen — Technical University of Denmark, Lyngby, Denmark

Atomically thin two-dimensional (2D) materials have recently emerged as a new class of materials with unique and highly tunable optoelectronic properties. Different 2D crystals can be stacked to form van der Waals heterostructures (vdWH) where the individual 2D layers are held together by weak van der Waals forces leading to atomically well-defined interfaces. This fascinating scenario opens up the possibility of designing heterostructures with tailored electronic or optical properties. I will give a general introduction to the electronic properties of 2D materials, including characteristic features of their dielectric screening and collective excitations with special emphasis on the challenges related to their ab-initio description. I will show how the dielectric function of a given 2D material can be controlled by embedding it into a vdWH, and how this in turn can be used to control the band structure, exciton binding energies or the plasmon dispersion in 2D materials.

TT 45.2 Wed 11:00 GER 38

Charge and energy transport at the nanoscale: A DFT perspective — •Florian G. Eich, Fabio Covito, and Angel Rubio — Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, D-22761 Hamburg, Germany

Understanding the interplay between charge and energy transport at the nanoscale paves the way for novel thermoelectric devices, which may prove useful for the development for sustainable energy sources. However, concepts, such as heat flow, temperature and entropy are only well-established at the macroscopic level for slow dynamics. This raises the question about whether these concepts can be employed for small length and short time scales. We will present our recent efforts to use a time-dependent density-functional theory framework, dubbed nonequilibrium thermal DFT, in order to generalize temperature and heat or energy flow to the microscopic regime. To this end we will highlight the analogy of the formally exact microscopic equations of motion for charge density and energy density in thermal DFT to the macroscopic equations of motion of hydrodynamics. Furthermore, we will present first result using our approach to compute transient energy energy currents induced by a temperature gradient and show that in the steady-state limit persistent temperature oscillations develop.

TT 45.3 Wed 11:15 GER 38

Conductance of aromatic and antiaromatic molecular circuits — Narendra P. Arasu and •Héctor Vázquez — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

Molecular structures with delocalized conjugated orbitals play an essential role in molecular transport due to their high conductance and small attenuation factors. While much work has been done on aromatic molecules, some studies have shown that conductance actually decreases with aromaticity [1].

In this talk I will discuss the effect of (anti)aromaticity on conductance. I will show results of first-principles transport calculations for an aromatic-antiaromatic pair of molecules and compare with experiment. Conductance is calculated using DFT and NEGF including corrections to the DFT level positions. The corrected conductance values are in very good agreement with experiment. We find that the conductance of the antiaromatic molecule is much higher than that of its aromatic counterpart. Calculations show this to be a consequence of the smaller HOMO-LUMO gap of the antiaromatic complex as well as on the molecular level alignment at the junction [2].

[1] W. Chen, H. Li, J.R. Widawsky, C. Appayee, L. Venkataraman, and R. Breslow, J. Am. Chem. Soc. 136 918 (2014).

[2] S. Marqués-González, S. Fujii, J.-Y. Shin, H. Shinokubo, N.P. Arasu, H. Vázquez and M. Kiguchi, (to be submitted).

TT 45.4 Wed 11:30 GER 38

Current-induced cooling of Carbene-based molecular junctions: role of electrodes structure — •Giuseppe Foti and Héctor Vázquez — Institute of Physics, Czech Academy of Sciences Cukrovarnicka 10, Prague 6

In this talk I will present our first principles calculations based on density functional theory (DFT) plus Nonequilibrium Green's functions (NEGF) of the current-induced heating and cooling dynamics of a series of Carbene-based molecular junctions [1]. I will show how the atomistic details of electrode terminations have a strong impact on the heating dynamics of the junctions and how they can maximize the cooling of the system. In the cases where the molecule is attached to blunt leads and the electronic coupling to bulk states is strong the cooling efficiency of the most active vibrational modes decreases monotonically as bias increases. This results in the heating of the junction. On the other hand, when the molecule is connected to sharp electrode terminations such as chain-like structures, which can be formed experimentally when the metal-molecule bond is mechanically strong, and the electronic coupling to electrode states is weak, the cooling efficiency shows a non-monotonic behavior. It first decreases as a function of voltage but then increases at relatively high biases, effectively cooling down the junction [2]. These results reveal the important role of the atomistic structure of metal-molecule interface in the current-induced damping of localized molecular vibrations.

[1] Foti, G.; Vázquez, H. Nanotechnology 2016, 27, 125702.

[2] Foti, G.; Vázquez, H. submitted

TT 45.5 Wed 11:45 GER 38

DFTB-based recursive Green's function algorithms for electron transport in quasi-1D systems — •Fabian Teichert[1,2,4], Andreas Zienert[3,4], Jörg Schuster[4], and Michael Schreiber[2] — [1]Dresden Center for Computational Materials Science (DCMS), Dresden, Germany — [2]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [3]Center for Microtechnologies (ZfM), Technische Universität Chemnitz, Chemnitz, Germany — [4]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Within the last decades, quantum transport theory and density functional theory have become very important for predicting the electronic properties of new materials and future electronic devices.

We focus on the problem of improving quantum transport algorithms for large quasi-1D systems which are enormously time-consuming today. We combine the density functional tight binding (DFTB) approach with the recursive Green's function formalism (RGF), which is very effective for such systems. First, we show how to improve the RGF for the case of randomly distributed real defects. For this, we use the steps of the renormalization decimation algorithm (RDA), which is part of the electrode calculation. Second, we show how to improve the calculation of the surface Green's functions of electrodes which have a long unit cell. Here, we employ the decimation technique to reduce the dimensionality of the periodic Hamiltonian matrix, leading to effective matrices, which are treated by the RDA. Finally, we apply these algorithms to carbon nanotubes and present our results.

TT 45.6 Wed 12:00 GER 38

Conditions for formation of two-dimensional electron gas at the $LaFeO_3/SrTiO_3$ — •Igor Maznichenko[1], Sergey Ostanin[1], Arthur Ernst[2], Ingrid Mertig[1,2], Katayoon Mohseni[2], Holger L. Meyerheim[2], Eberhard K.U. Gross[2], Pengfa Xu[3], Wei Han[3], Philip M. Rice[3], Jaewoo Jeong[3], Mahesh G. Samant[3], and Stuart S.P. Parkin[2,3] — [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 — [3]IBM Almaden Research Center, 650 Harry Road, San Jose, California 95120, USA

The formation of a conducting two dimensional electron gas (2DEG) at the interface between two insulating oxide layers was explained theoretically for atomically and chemically abrupt interfaces via polar discontinuity.

Here we show that a 2DEG is formed at the interface between thin layers of lanthanum ferrite, $LaFeO_3$ (LFO), that are more than 3 unit cells thick, when grown epitaxially on $SrTiO_3$ (STO) (001). The interface property highly depends on the surface property of TiO_2 terminated STO. The interface is conducting if the STO is not annealed in an oxygen environment prior to the LFO growth, while insulating if the STO is annealed.

First principles calculations reveal that a 2DEG should be realized for an ideal interface but that modest chemical intermixing suppresses it. These calculations also show that the presence of oxygen vacancies supports 2DEG formation due to electronic doping.

TT 45.7 Wed 12:15 GER 38

Thermal Renormalization of the Electronic Structure: Trends across Chemical and Structural Space — •Honghui Shang[1], Christian Carbogno[1], Patrick Rinke[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Aalto University, Helsinki, Finland

Advances in electronic structure theory now allow us to compute the renormalization of the electronic structure due to thermal nuclear motion from first principles [1]. In this work, we present a systematic computational assessment of this renormalization for 82 octet binaries in both the zincblende and the rocksalt structure. After validating our computational approach that is based on finite-differences [2] and Fröhlich-type corrections [3] for polar materials, we discuss and analyze the observed trends: For instance, we find that most materials exhibit the expected band-gap reduction upon temperature increase; however, some materials (e.g. CuCl and CdO) do not follow this trend and exhibit the opposite behavior. We discuss the underlying electronic mechanism as well as its dependence on the chemical composition and structure of the material. In this context, also the sensitivity of such calculations with respect to the chosen basis set and exchange-correlation functional (LDA, PBE, HSE06) are critically investigated.
[1] F. Giustino, arXiv:1603.06965 (2016).
[2] G. Antonius, *et al. Phys. Rev. Lett.* **112**, 215501 (2014).
[3] J. P. Nery and P. B. Allen, *Phys. Rev. B* **94**, 115135 (2016).

TT 45.8 Wed 12:30 GER 38

Spin-wave excitations and electron-magnon scattering from 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

We study the spin excitations and the electron-magnon scattering in bulk Fe, Co, and Ni within the framework of many-body perturbation theory as implemented in the full-potential linearized augmented-plane-wave method. Starting from the *GW* approximation we obtain a Bethe-Salpeter equation for the magnetic susceptibility treating single-particle Stoner excitations and magnons on the same footing. 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 theorem and present an approach that implements the magnetic susceptibility using a renormalized Green function instead of the non-interacting one, leading to a substantial improvement of the Goldstone-mode condition [1]. Finally, we employ the solution of the Bethe-Salpeter equation to construct a self-energy that describes the scattering of electrons and magnons. The resulting renormalized band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy. We also see kinks in the electronic bands, which we attribute to electron scattering with spatially extended spin waves.
[1] Müller *et al.*, Phys. Rev. B **94**, 064433 (2016).

TT 45.9 Wed 12:45 GER 38

Charged supercells revised: Small Polarons in Oxides with proper account for long-range polarization — •Sebastian Kokott, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, DE

Formation of small polarons (excess charges localized within one unit cell) often determines charge mobility and optical absorption in oxide materials. In this work, we address two important challenges in the DFT description of small polarons: sensitivity to the errors in exchange-correlation (XC) treatment and finite-size effects in supercell calculations. The polaron properties are obtained using a modified neutral potential-energy surface (PES) [1]. Using the hybrid HSE functional and considering the whole range $0 \leq \alpha \leq 1$ of exact exchange, we show that the modified PES model significantly reduces the dependence of the polaron level and binding energy in MgO and TiO_2 on the XC treatment. It does not eliminate the dependence on supercell size. Based on Pekar's model [2], we derive the proper long-range behavior of the polaron and a correction that allows to obtain the polaron properties in the dilute limit (tested for supercells containing up to 1,000 atoms). The developed approach reduces drastically the computational time for exploring the polaron PES, and gives a consistent description of polarons for the whole range of α. It allows us to find a self-trapped hole in MgO that is noticeably more stable than reported previously.—[1] B. Sadigh *et al.*, PRB **92**, 075202 (2015); [2] S.I. Pekar, ZETF **16**, 335 (1946). This work received funding from the Leibniz ScienceCampus "GraFOx".

TT 46: Focus Session: Collective Quantum Dynamics: From Fundamentals to New Phenomena

This session covers recent experimental and theoretical advances both in condensed mater physics as well as in cold atomic systems in the field of dynamical and nonequilibrium properties of quantum many-body systems. Collective quantum dynamics plays a central role in a number of different physical systems. First, dynamical systems will exhibit a rich set of phenomena which lie beyond static ground state properties, e.g. in non-thermal many-body localised systems. Second, dynamical properties of many-body systems can serve as experimentally accessible probes to detect characteristic fingerprints of otherwise featureless phases of matter, such as topologically ordered and fractionalized states of matter. Recent technological advances have had an impact on all of these aspects of the field, while continuing experimental progress in AMO and materials physics is valuable in providing access to new phenomena, as well as testing new theoretical findings.

Organization: Frank Pollmann, MPI-PKS, Dresden; Roderich Moessner, MPI-PKS, Dresden

Time: Wednesday 15:00–17:45 Location: HSZ 03

Invited Talk TT 46.1 Wed 15:00 HSZ 03

Many-Body Localization and Glassiness in Quantum Spin Systems — •Antonello Scardicchio — Abdus Salam ICTP, Trieste, Italy — INFN, Sezione di Trieste, Trieste, Italy

I will discuss the interplay of two phenomena arising in disordered quantum spin systems: the appearance of a glassy phase, and the complete suppression of transport due to many-body localization. I will review work done on some models, under various approximations (analytical and numerical), and summarize a universal physical picture for how the two dynamical phases can interplay. I will also comment on the implications for the performance of quantum computers.

Invited Talk TT 46.2 Wed 15:30 HSZ 03

Exploring Many-Body Localization in Two Dimensions — •Christian Gross — Max-Planck-Institut für Quantenoptik, Garching

The question of thermalization in closed quantum systems is currently a topic of intense research and ultracold atoms are an almost ideal experimental system for its study. In this context it is particularly interesting to study systems that do not thermalize. Many-body localized systems form a generic class of such systems, which is largely unexplored in higher dimensions and at high energy densities. Here we report on recent experiments with single site resolved ultracold lattice bosons in two dimensions subject to random disorder. Our data

indicates a transition from thermalizing behavior at low disorder to localization at higher disorder and a diverging length scale at the transition. Finally we discuss ongoing experimental effort and possibilities to characterize the MBL phase close to the transition point.

Invited Talk TT 46.3 Wed 16:00 HSZ 03

Floquet Engineering and Control of Topology in Solid State Systems — •Takashi Oka[1,2], Leda Bucciantini[1,2], Sthitadhi Roy[2], and Sota Kitamura[3] — [1]Max Planck institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck institute for Chemical Physics of Solids, Dresden, Germany — [3]The university of Tokyo, Department of Tokyo, Tokyo, Japan

Periodically driven quantum system is attacting interest as a way to create new state of matter with exotic topological and dynamical properties.

1. Emergent Weyl points and Fermis arcs in a Floquet Weyl semimetal [1]: We find that a series of infinite numbers of Weyl points emerges, moves and annihilates in a Floquet Weyl semimetal that can be realized by applying circularly polarized laser to a three dimensional Dirac mateiral.

2. Landau quantization in an oscillating magnetic field [2]: We find that Landau quantization is not restricted to a static magnetic field but can be realized in oscillating fields and find a state that is analogous to the integer quantum Hall effect (QHE) when the ratio between the cyclotron frequency and the laser frequency is given by magic numbers.

[1] L. Bucciantini, S. Roy, S. Kitamura, and T. Oka, in prep.
[2] T. Oka, and L. Bucciantini, Phys. Rev. B 94, 155133 (2016)

15 min. break.

Invited Talk TT 46.4 Wed 16:45 HSZ 03

Hydrodynamic Regimes of Electron Transport — •Andrew Mackenzie — Max Planck Institute for Chemical Physics of Solids, Nöthnitzerstr 40, Dresden

In this talk I will discuss recent experiments showing that in some ultra-pure metals, it is possible to reach a regime of transport in which the viscosity of the electronic fluid plays a significant role in determining its flow. The conditions for this to happen are rather stringent, but there is some prospect of achieving them in a broader range of materials than those so far studied, so I will also try to give a sense of the future directions that the field might take.

Invited Talk TT 46.5 Wed 17:15 HSZ 03

Dynamical Phase Transitions — •Stefan Kehrein — Univ. Göttingen

Phase transitions play a central role in the theory of equilibrium statistical mechanics. They are indicated by non-analytic behavior of the free energy in the thermodynamic limit, for example at a critical temperature. The goal to understand and classify equilibrium phase transitions led to the fundamental concept of universality with its far-reaching implications in many different fields of physics.

Interestingly, similar non-analytic behavior of the dynamical free energy at certain critical times has been found in the real time evolution of the quantum Ising model [1]. This behavior has been denoted dynamical phase transition and has since been theoretically investigated in numerous other non-equilibrium quantum many-body models. Recently, the first experimental observation of dynamical phase transitions was reported in an ultracold fermionic quantum gas that was quenched between a static and a Floquet Hamiltonian [2].

This talk will give an overview over the current theoretical understanding of such dynamical phase transitions, the role of non-zero temperature and non-integrable perturbations, and possible experimental verifications.

[1] M. Heyl, A. Polkovnikov, and S. Kehrein, Phys. Rev. Lett. 110, 135704 (2013)
[2] N. Fläschner, D. Vogel, M. Tarnowski, B. S Rem, D.-S. Lühmann, M. Heyl, J. C. Budich, L. Mathey, K. Sengstock, and C. Weitenberg, arXiv:1608.05616

TT 47: Superconductivity: Properties and Electronic Structure 2

Time: Wednesday 15:00–18:00 Location: HSZ 103

Invited Talk TT 47.1 Wed 15:00 HSZ 103

Interplay between CDW and Superconductivity: Effect of Pressure — •Matthieu Le Tacon — Karlsruher Institut für Technologie, Institut für Festkörperphysik, D-76021 Karlsruhe, Deutschland

I will focus on the interplay between superconductivity and charge density waves in superconducting cuprates and dichalcogenides. High resolution inelastic x-ray scattering was used to observe of a quasi-elastic *central peak* in underdoped $YBa_2Cu_3O_{6.6}$, demonstrating the static nature of the CDW correlations, attributed to the pining of CDW nanodomains on defects. Low energy phonons also exhibit anomalously large superconductivity induced renormalizations close to the CDW ordering wave vector, providing new insights regarding the long-standing debate of the role of the electron-phonon interaction, a major factor influencing the competition between collective instabilities in correlated-electron materials. Relationship to the well-known anomalies in reported in the higher energy phonon branches will be discussed. Finally, the dependence of these effects with pressure will be reported.

Pressure has also been used to tune the ground state of a less correlated material, 2H-$NbSe_2$. There a fast hardening of the soft phonon mode with pressure is observed, much faster than predicted by calculations carried out at the harmonic level. The inclusion of the full anharmonic potential in the calculation yields an excellent agreement with the experimental data and further allows demonstrating the major role of the electron-phonon interaction in the superconducting mechanism.

TT 47.2 Wed 15:30 HSZ 103

Thermodynamic and Raman study of untwinned $La_{1.8-x}Eu_{0.2}Sr_xCuO_4$ single crystals — •Julia Martius[1], Liran Wang[1], Peter Adelmann[1], Michael Merz[1], Frédéric Hardy[1], Mingquan He[1], Matteo Minola[2], Tomohioro Takayama[2], Hidenori Takagi[2], Christoph Meingast[1], and Matthieu Le Tacon[1] — [1]Institute for Solid-State Physics, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany. — [2]Max-Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart Germany.

Partial substitution of La by Eu in $La_{2-x}Sr_xCuO_4$ leads to a stabilization of a low-temperature-tetragonal (LTT) phase, in which superconductivity is strongly suppressed at a doping of x = 1/8 [1]. This suppression has been attributed to long-range charge and magnetic ordering, which in $La_{1.8-x}Eu_{0.2}Sr_xCuO_4$ have been reported to occur at around 80 K and 30 K, respectively, i.e. well below the LTT transition at 130 K [2]. In this study we have looked for thermodynamic signatures of these ordering phenomena in high-quality untwinned single crystals using high-resolution thermal-expansion, specific-heat and magnetization measurements. The thermodynamic data are supplemented by electronic Raman measurements.

[1] B. Büchner *et al.*, Phys. Rev. Lett. 73, 1841 (1994).
[2] J. Fink *et al.*, Phys. Rev. B 83, 092053 (2011).

TT 47.3 Wed 15:45 HSZ 103

Changing the Start-point in the Cuprates — •Carsten Putzke — University of Bristol

Far over-doped $Tl_2Ba_2CuO_{6+\delta}$ is one of the cleanest and best understood members of the cuprate family. In this material quantum oscillation, specific heat and Hall effect measurements show good agreement with one another as well as band structure calculations. Choosing this as a start-point and reducing the oxygen stoichiometry enables to tune this system from far over-doped ($T_c < 4.2\,\mathrm{K}$) to optimal doping ($T_c = 94\,\mathrm{K}$) and even into the under-doped region. Thereby covering the entire over-doped part of the phase diagram. This proves particularly interesting as it allows us to study electronic correlation without the complication of the manifold ground states observed in the underdoped part of the phase diagram.

Starting from a Fermi-liquid like behaviour in far over-doped samples I will show results of the magnetoresistance and Hall effect in pulsed magnetic field that demonstrate the evolution of the electronic properties upon approaching the highest critical temperature in the system and the deviations from this evolution that accompany the entrance to the under doped regime.

TT 47.4 Wed 16:00 HSZ 103

Magnetic Flux Distribution in YBCO Thin Films Investigated via XMCD Microscopy at Low Temperatures — •Julian Simmendinger[1], Claudia Stahl[1], Stephen Ruoss[1], Markus Weigand[1], Gisela Schütz[1], and Joachim Albrecht[2] — [1]Max-Planck-Institute for Intelligent Systems, Heisenbergstraße 3, 70569 Stuttgart, Germany — [2]Research Institute for Innovative Surfaces, FINO, Aalen University, Beethovenstraße 1, 73430 Aalen

The magnetic flux distribution of high-T_c $YBa_2Cu_3O_{7-\delta}$ (YBCO) thin films exhibits structures within the submicrometer regime. Therefore scanning x-ray microscopy based on the x-ray magnetic circular dichroism effect (XMCD) is our method of choice revealing very high spatial resolution of both surface structure and magnetization distribution [1,2]. Introducing an XMCD sensitive, soft-magnetic CoFeB respectively Py sensor layer wherein the magnetic stray field of the superconductor is mapped [3], the critical current density and its dependency of the defect structure in the YBCO thin films are imaged and analyzed.

The measurements were carried out at the scanning x-ray microscope MAXYMUS at Bessy II, HZB Berlin utilizing a new low temperature setup.

[1] S. Ruoß et al., Appl. Phys. Lett. 106, 022601 (2015).
[2] S. Ruoß et al., New J. Phys. 18, 103044 (2016).
[3] C. Stahl et al., J. Appl. Phys. 117, 17D109 (2015).

TT 47.5 Wed 16:15 HSZ 103

Detailed analysis of magnetization loops of electrospun nonwoven superconducting fabrics — •XianLin Zeng[1], Denis Gokhfeld[2], Thomas Karwoth[1], Michael Koblischka[1], Thomas Hauet[3], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany — [2]Kirensky Institute of Physics, Siberian Branch of the Russian Academy of Sciences, Akademgorodok 50/38, Krasnoyarsk, 660036 Russia — [3]Kirensky Institute of Physics, Siberian Branch of the Russian Academy of Sciences, Akademgorodok 50/38, Krasnoyarsk, 660036 Russia

Networks of superconducting $Bi_2Sr_2CaCu_2O_8$ (Bi-2212) nanowires were fabricated by the electrospinning technique. The nanowires form a non-woven, fabric-like network with numerous interconnects enabling a current flow between the nanowires. The porosity of this nanowire network is 0.9928. Therefore, this material represents a novel class of ultraporous high-temperature superconductors. The magnetization of the nanowire networks were recorded by SQUID magnetometry. The magnetic properties were analyzed using the extended critical state model (ECSM). Single nanowires have remarkably high values of the critical current density of 1.69×10^7 A/cm^2 at 5 K. The resulting sample critical current density of 7.44×10^4 A/cm^2 at 5 K is fine for this lightweight material. Using the ECSM, several important magnetic parameters could be determined including the penetration field, H_p, the irreversibility fields, H_{irr}, the upper critical field, H_{c2}, and the flux pinning forces.

15 min. break.

TT 47.6 Wed 16:45 HSZ 103

Heat Capacity Measurements of Sr_2RuO_4 Under Uniaxial Stress — •You-Sheng Li[1,2], Alexandra Gibbs[3], Andrew Mackenzie[1,2], Clifford Hicks[1], and Michael Nicklas[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]University of St. Andrews, School of Physics and Astronomy, United Kingdom — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany

One of the most-discussed possible pairing symmetries of the superconductor Sr_2RuO_4 is $p_x \pm ip_y$. By applying in-plane uniaxial stress, the degeneracy of the p_x and p_y components should be lifted, yielding two critical temperatures (T_c). Hicks et al. observed an increase of T_c of Sr_2RuO_4 under both compressive and tensile stress [1], and did not find evidence for splitting of transition. However, that result was based on magnetic susceptibility measurements, which would be sensitive only to the upper transition. For a direct test of possible splitting, we measure the heat capacity of Sr_2RuO_4 under uniaxial stress. To do so, we have developed an approach to measure heat capacity under non-adiabatic conditions. We have observed the increase in T_c under compressive strain, providing the first thermodynamic evidence for the strain-induced increase in T_c of Sr_2RuO_4, and also resolve strong strain-induced changes in the normal-state heat capacity.

[1] Clifford W. Hicks et al., Science 344, 283 (2014).

TT 47.7 Wed 17:00 HSZ 103

Upper Critical Field of Strained and Unstrained Sr_2RuO_4 — •Fabian Jerzembeck[1], Alexander Steppke[1,2], Mark E. Barber[1,2], Alexandra S. Gibbs[2,3], Yoshiteru Maeno[4], Andrew P. Mackenzie[1,2], and Clifford W. Hicks[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Scottish Universities Physics Alliance (SUPA), School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom — [3]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot OX11 OQX, United Kingdom — [4]Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan

The dependence of the upper critical field H_{c2} of a superconductor on temperature can provide information on structure of the gap. We have recently shown that T_c of the unconventional superconductor Sr_2RuO_4 can be dramatically enhanced by uniaxial pressure, most likely due to tuning one of the Fermi surfaces through a Lifshitz transition. We have also shown that the form of $H_{c2}(T)$ is very different between unstressed and highly-stressed Sr_2RuO_4. In this talk, we present further data on H_{c2} of stressed and unstressed Sr_2RuO_4, and discuss how pressure is modifying the gap.

[1] A. Steppke et al. arXiv:1604.06669

TT 47.8 Wed 17:15 HSZ 103

Microwave spectroscopy on superconducting Nb:$SrTiO_3$ at mK temperatures — •Markus Thiemann[1], Manfred Beutel[1], Evangelos Fillis-Tsirakis[2], Hans Boschker[2], Jochen Mannhart[2], Martin Dressel[1], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Max Planck Institute for Solid State Research, Stuttgart

Niobium-doped $SrTiO_3$ (Nb:STO) is a superconductor, exhibiting the lowest charge carrier density among all superconductors. It shows a dome in the transition temperature as a function of doping concentration with a maximum $T_c \approx 0.4$ K. Early tunneling experiments as well as more recent quantum oscillation measurements suggested Nb:STO being a multiband superconductor. Since the low intrinsic energy scales of the system are within the GHz range, microwave spectroscopy is the adequate contactless technique to reveal the intrinsic electronic properties of this system.

We performed microwave measurements on Nb:STO across the superconducting dome, using superconducting stripline resonators. We were able to determine the complex optical conductivity covering a temperature and frequency range of 70-500 mK and 1-20 GHz. From the complex conductivity we determined the temperature dependence of the superfluid density and superconducting energy gap. Both, as well as the frequency dependence of the complex conductivity can be described well with a single band BCS-model contradicting the multiband hypothesis.

TT 47.9 Wed 17:30 HSZ 103

Paramagnetic Meissner effect in topological superconductor candidate $Sr_xBi_2Se_3$ — •zhiwei wang[1], ruixing zhang[2], alexey taskin[1], huaixin yang[2], jianqi li[2], and yoichi ando[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Institute of Physics, Chinese Academy of Science, 100190, Beijing, P. R. China

Single crystals of superconducting $Sr_xBi_2Se_3$ with the actual Sr content up to $x = 0.14$ have been grown. The highest $T_c = 3.12$ K has been observerd in $x = 0.048$ sample in electrical transport measurment and it dereases with the increase of actual Sr content. The highest superconducting volume fraction is close to 100% determined from magnetic susceptibility measurement at 1.75 K. An unexpected paramagnetic Messner effect (PME) has been observed in all measured $Sr_xBi_2Se_3$ samples at lower magnetic fields. We attribute this PME to imhomogeneous microstructure of $Sr_xBi_2Se_3$, which was supported by transmission eletron microscope (TEM) analysis. In addition, resistive transitions under magnetic fields point to an unconventional temperature dependence of the upper critical field B_{c2}.

TT 47.10 Wed 17:45 HSZ 103

topological quantum phase transition and superconductivity induced by pressure in the bismuth tellurohalide BiTeI — •Yanpeng Qi[1], Wujun Shi[1,2], Pavel G. Naumov[1], Nitesh Kumar[1], Raman Sankar[3,4], Walter Schnelle[1], Chandra Shekhar[1], F. C. Chou[4], Claudia Felser[1], Binghai Yan[1,2,5],

and Sergey A. Medvedev[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]School of Physical Science and Technology, ShanghaiTech University, Shanghai 200031, China — [3]Institute of Physics, Academia Sinica, Taipei 10617, Taiwan. — [4]Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan. — [5]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany.

A pressure-induced topological quantum phase transition has been theoretically predicted for the semiconductor BiTeI with giant Rashba spin splitting. In this work, the evolution of the electrical transport properties in BiTeI and BiTeBr is investigated under high pressure. The pressure-dependent resistivity in a wide temperature range passes through a minimum at around 3 GPa, indicating the predicted transition in BiTeI. Superconductivity is observed in both BiTeI and BiTeBr while the resistivity at higher temperatures still exhibits semiconducting behavior. Theoretical calculations suggest that the superconductivity may develop from the multi-valley semiconductor phase. The superconducting transition temperature Tc increases with applied pressure and reaches a maximum value of 5.2 K at 23.5 GPa for BiTeI (4.8 K at 31.7 GPa for BiTeBr), followed by a slow decrease.

TT 48: Superconductivity: Tunnelling, Josephson Junctions, SQUIDs 2

Time: Wednesday 15:00–17:45 Location: HSZ 201

TT 48.1 Wed 15:00 HSZ 201

Josephson parametric amplifier with mixing of three traveling waves — •Alexander B. Zorin, Judith Dietel, Ralf Dolata, and Marat Khabipov — Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

Due to accessible quantum-limited performance Josephson parametric amplifiers are important tools in quantum information technology and the traveling-wave Josephson parametric amplifiers with inherently large bandwidth are especially desired for fast signal processing and frequency multiplexing. So far these devices have required the four-wave mixing condition to operate and special compensation of unavoidable phase mismatch [1,2]. We show, however, that there is an elegant way to realize efficient three-wave mixing at negligible phase mismatch without applying sophisticated dispersion engineering. Our Josephson traveling-wave parametric amplifier is based on a chain of rf-SQUIDs forming a metamaterial transmission line possessing quadratic nonlinearity [3]. It can have large (exponential) gain, wide bandwidth, and ultimately quantum-limited characteristics, outperforming its state-of-the-art four-wave counterparts. Recent experimental data obtained with first Nb circuits at temperature $T = 4.2$ K will also be reported.

[1] T. C. White *et al.*, Appl. Phys. Lett. **106**, 242601 (2015).
[2] C. Macklin *et al.*, Science **350**, 307 (2015).
[3] A. B. Zorin, Phys. Rev. Applied **6**, 034006 (2016).

TT 48.2 Wed 15:15 HSZ 201

Superconducting nanowire loop capacitively coupled to a microwave resonator — •Hannes Rotzinger[1], Sebastian T. Skacel[1], Jochen Braumüller[1], Andre Schneider[1], Hans Mooij[2], and Alexey V. Ustinov[1] — [1]Karlsruher Institut für Technologie, Karlsruhe, Deutschland — [2]Kavli Institute of NanoScience, Delft, the Netherlands

We present continuous and pulsed microwave measurements of a high-impedance superconducting loop with an embedded superconducting nanowire of 20 nm width and 250 nm length. In the experiment, we monitor the dispersive shift of a microwave resonator which couples capacitively to the loop. When applying weak magnetic fields, the system shows pronounced anti-crossings at the resonator frequency that occur at stable and reproducible fields. At larger fields, the anti-crossings are shifted hysteretically by magnetic flux values comparable to the magnetic flux quantum per loop area. We analyse the anti-crossings by two-tone measurements and find signatures of several specific two-level states at different magnetic fields. Rabi oscillations as well as T1 and T2 coherence times are measured by applying microwave pulses.

TT 48.3 Wed 15:30 HSZ 201

A niobium based three-axis vector nanoSQUID — •Katrin Meyer[1], Maria José Martínez-Pérez[1], Benedikt Müller[1], Diego Gella[1], Viacheslav Morosh[2], Thomas Weimann[2], Roman Wölbing[1], Javier Sesé[3], Oliver Kieler[2], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Germany — [2]Fachbereich Quantenelektronik, Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [3]Laboratorio de Microscopías Avanzadas (LMA), Instituto de Nanociencia de Aragón (INA), Universidad de Zaragoza, Spain

We present the design, realization, and performance of 3-axis vector nanoSQUIDs [1]. They consist of three mutually orthogonal SQUID nanoloops (two magnetometers, one gradiometer) that allow simultaneous and independent detection of the three components of the vector magnetic moment of individual magnetic nanoparticles (MNPs). All three nanoSQUIDs are realized within an area of a few μm^2 on a single chip. The devices are based on intrinsically shunted Nb/HfTi/Nb Josephson junctions and exhibit linewidths of ~ 250 nm. Operation at 4.2 K in external magnetic fields up to ~ 50 mT is demonstrated, with a flux noise below $\sim 250\,\mathrm{n}\Phi_0/\mathrm{Hz}^{1/2}$ in the white noise limit. Depending on device geometry and MNP position, spin sensitivities down to below $100\,\mu_\mathrm{B}/\mathrm{Hz}^{1/2}$ are achieved. We also present approaches to extend operation to larger external magnetic fields and to improve the spin sensitivity.

[1] M. J. Martínez-Pérez *et al.*, ACS Nano **10**, 8308–8315 (2016).

TT 48.4 Wed 15:45 HSZ 201

NanoSQUID magnetometry of individual cobalt nanoparticles — •Benedikt Müller[1], Maria José Martínez-Pérez[1], Dennis Schwebius[1], Dana Korinski[1], Jianxin Lin[1], Reinhold Kleiner[1], Javier Sesé[2], and Dieter Koelle[1] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Germany — [2]Laboratorio de Microscopías Avanzadas (LMA), Instituto de Nanociencia de Aragón (INA), Universidad de Zaragoza, Spain

We demonstrate the operation of low-noise nanoSQUIDs based on the high critical field and high critical temperature superconductor $YBa_2Cu_3O_7$ (YBCO) as ultra-sensitive magnetometers for single magnetic nanoparticles (MNPs) [1]. The nanoSQUIDs contain grain boundary Josephson junctions and are patterned by focused ion beam milling. They can be operated over extremely broad ranges of applied magnetic field (up to ~ 1 T) and temperature ($0.3\,\mathrm{K} < T < 80\,\mathrm{K}$). Cobalt MNPs with typical size of several tens of nm have been grown directly on top of the sensors by focused electron beam induced deposition. This allows us to investigate the magnetization reversal of individual MNPs with magnetic moments $(1-30)\times10^6\mu_\mathrm{B}$. The magnetization reversal appears to be thermally activated over an energy barrier, which has been quantified for the (quasi) single-domain particles. These measurements demonstrate that YBCO nanoSQUIDs are exceptional magnetometers for the investigation of individual nanomagnets.

[1] M. J. Martínez-Pérez *et al.*, Supercond. Sci. Technol. **30**, 024003 (2016)

TT 48.5 Wed 16:00 HSZ 201

Charge QUantum Interference Device (CQUID) — Sebastian E. de Graaf[1], •Sebastian T. Skacel[2], Teresa Hoenigl-Decrinis[1,3], Rais Shaikhaidarov[3,4], Hannes Rotzinger[2], Sven Linzen[5], Mario Ziegler[5], Vladimir Antonov[3,4], Evgeni Il'ichev[5,6], Alexey V. Ustinov[2,6], Alexander Ya. Tzalenchuk[1,3], and Oleg A. Astafiev[1,3,4,6] — [1]National Physical Laboratory, Teddington, UK — [2]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Germany — [3]Department of Physics, Royal Holloway University of London, Egham, UK — [4]Moscow Institute of Physics and Technology, Moscow, Russia — [5]Leibniz Institute of Photonic Technology, Jena, Germany — [6]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia

Quantum mechanics postulate a duality between magnetic flux and electric charge in superconducting devices. We present the experimental realisation of the Charge QUantum Interference Device (CQUID), exactly dual to the conventional Superconducting QUantum Interfer-

ence Device (SQUID). The CQUID is made out of 3.3 nm thin Atomic Layer Deposited superconducting NbN film. Two narrow constrictions connected in series via a small island act as barriers for flux tunnelling across the superconductor, carried by quantum phase slips. A gate electrode can tune the charge induced on the island, making the CQUID a charge sensitive interferometer based on the Aharonov-Casher effect. We demonstrate control of flux tunnelling interference across a continuous superconductor by an induced charge.

15 min. break.

TT 48.6 Wed 16:30 HSZ 201

Recent insights in low-frequency excess flux noise of superconducting quantum devices — •Sebastian Kempf, Anna Fering, David Uhrig, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

Low-frequency excess flux noise strongly diminishes the performance of flux-sensitive superconducting quantum devices. It limits, for example, the coherence time of flux and phase qubits and makes SQUID based measurements of low-frequency signals challenging. Recent experiments suggest that low-frequency excess flux noise in Josephson junction based devices originates from the random reorientation of interacting spins located in surface layer oxides or in the interface between the substrate and the device wiring. Though this explanation proves to be generally correct, the physical nature of these spins, i.e. their origin as well as their interaction mechanisms, has not be been resolved so far and many questions remain.

In this contribution we present a comprehensive analysis of low-frequency excess flux noise. Our analysis include 373 individual noise spectra that were taken from 84 superconducting quantum devices at temperatures below 1 K. It revealed an evidence for a material and device type dependence of low-frequency excess flux noise and showed that SQUID arrays systematically feature higher noise exponents than single SQUIDs. This somehow facilitates to engineer the shape of magnetic flux noise spectra by choosing a proper device material and type.

TT 48.7 Wed 16:45 HSZ 201

Transmission-Line Resonators for the Study of Individual Two-Level-Systems — •Jan Brehm, Alexander Bilmes, Alexey V. Ustinov, and Jürgen Lisenfeld — Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Parasitic Two-Level-Systems (TLS) arise from microscopic material defects and are one of the main sources of decoherence in superconducting devices such as SQUIDs, resonators and quantum bits (qubits). The high sensitivity of quantum circuits motivates one to build a universal detector for single TLS, which can be applied to various materials. Josephson junction based superconducting qubits, e.g., offer the possibility to resonantly drive individual TLS' and to observe their quantum dynamics using the qubit for TLS readout. Yet, those experiments have been restricted to TLSs hosted in the dielectric tunnel barrier of the qubit's Josephson junctions, which reduces the choice of explorable materials to few dielectrics. Here we show how TLS in thin films can be studied using a superconducting coplanar notch-type resonator whose end is terminated by a capacitor containing TLS in its insulating layer. By tuning TLS via mechanical strain, we observe the signatures of individual strongly coupled TLS in the resonator's reflection spectrum and noise characteristics.

TT 48.8 Wed 17:00 HSZ 201

Finding the Location of Two-Level-Systems within the Josephson Junction of a Superconducting Qubit — •Alexander Bilmes[1], Sebastian Zanker[2], Andreas Heimes[2], Michael Marthaler[2], Gerd Schön[2], Georg Weiss[1], Alexey V. Ustinov[1,3], and Jürgen Lisenfeld[1] — [1]Physikalisches Institut, KIT, 76131 Karlsruhe, Germany — [2]Institut für Theoretische Festkörperphysik, KIT, 76131 Karlsruhe, Germany — [3]Russian Quantum Center, MISIS, Moscow 119049, Russia

Superconducting quantum circuits represent the first solid state quantum bits that are close to fulfilling all criteria to realize a quantum processor. However, a severe coherence-limiting factor have been Two-Level-Systems (TLS) that reside in dielectric layers such as surface-oxides and the tunnel barrier of the junction. The strong coupling of junction-hosted TLS by their electrical dipole moment to the qubit enables us to apply resonant microwave pulses to the circuit and to observe the quantum state evolution of individual TLSs, while the qubit serves for TLS-readout. Such experiments reveal microscopic properties of single TLS and offer possible clues to reduce their impact on the qubit's quality. In a recent experiment we showed that TLS couple to evanescent electronic wave-functions leaking from the junction electrodes into the dielectric: Once the superconducting system is brought out of equilibrium, the TLS' energy relaxation is enhanced by inelastic scattering of BCS-quasiparticles. We exploit this interaction scheme to estimate the TLS' position across the tunnel barrier, providing valuable information at which fabrication step TLS preferably emerge.

TT 48.9 Wed 17:15 HSZ 201

Dielectric properties of disordered thin-film AlO_x — •Arnold Seiler[1], Saskia Meissner[1], Hannes Rotzinger[1], Stefan Fritz[2], and Georg Weiss[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie — [2]Laboratorium für Elektronenmikroskopie, Karlsruher Institut für Technologie

The nature of atomic tunneling systems (TS) in disordered thin-film dielectric aluminium oxide layers is of great interest. Combined investigation of a variety of fabrication techniques, microstructure analysis of the resulting material, particularly HR-TEM, and measurements of the bulk dielectric properties may give a hint on the nature of the defects.

In this report dielectric measurements in a wide frequency range are presented in order to shed light on the distribution of tunneling systems in AlO_x thin-films and their relaxation to phonons.

Resonant absorption for selected frequencies in the range of 1-6GHz yield the TS density in narrow bands whereas the temperature dependence of the dielectric function gives information on a broad energy range of TS. In the kHz frequency range the application of a magnetic field has a large impact on the dielectric properties which may be a hint that the TS are preferrably located close to the electrodes and interact with quasiparticles.

TT 48.10 Wed 17:30 HSZ 201

Quasiclassical Green's Function Approach to Normal-Metal Quasiparticle Traps — •Raphael Schmit and Frank Wilhelm-Mauch — Saarland University, Theoretical Physics Department

Superconducting qubits, such as the charge or the flux qubit, are thought to store the information needed for quantum information processing. However, unwanted interactions with the qubit's environment lead to decoherence of the qubit and thus information loss. In addition to these extrinsic sources for decoherence, there is also an intrinsic one: the coupling between the qubit and the non-equilibrium quasiparticle excitations in the superconductor the qubit is made of. Decoherence is due to quasiparticle tunneling through a Josephson junction, but there is also an inhomogeneous broadening caused by changes in the occupations of Andreev states in the junction. Both mechanisms are highly depending on the location of the quasiparticles: quasiparticles far away from junctions have much less contribution to decoherence than the ones close to it. While it is difficult to prevent the generation of quasiparticles, trapping them in less active regions of the device seems to provide a practicable way to improve the device performance.

We are aiming to establish a quantitative theory of normal-metal traps simply consisting of an island of normal metal which is in contact with the superconductor. To do so, we are applying a Green's function formalism - the Keldysh technique in the dirty limit with a quasiclassical approximation - to investigate the properties of non-equilibrium quasiparticles in mesoscopic devices.

TT 49: Transport: Topological Semimetals 2 (jointly with DS, MA, HL, O)

Time: Wednesday 15:00–17:45 Location: HSZ 204

TT 49.1 Wed 15:00 HSZ 204

Topological properties of magnetic semi-metals with non-symmorphic symmetries — •Andreas P. Schnyder — Max Planck Institute of Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart

Topological semi-metals exhibit band crossings near the Fermi energy, which are protected by the non-trivial topological character of the wave functions. In many cases, these topological band degeneracies give rise to exotic surface states and unusual magneto-transport properties. In this talk, I will discuss this physics in the context of *magnetic* semi-metals with non-symmorphic symmetries. In particular, I will show that non-symmorphic symmetries of cubic magnetic space groups lead to protected four-fold degenerate Dirac points and Dirac lines. As a concrete example, I will examine the topological properties of the antiferromagnet $CuBi_2O_4$ in terms of a low-energy tight-binding model, derived from ab-initio DFT calculations. I will discuss the monopole charges and the associated surface states of this system.

TT 49.2 Wed 15:15 HSZ 204

Density wave instabilities and surface state evolution in interacting Weyl semimetals — Manuel Laubach[1], Christian Platt[2], Ronny Thomale[3], Titus Neupert[4], and •Stephan Rachel[1] — [1]TU Dresden — [2]Stanford University — [3]University of Würzburg — [4]University of Zürich

We investigate the interplay of many-body and band structure effects of interacting Weyl semimetals (WSM). Attractive and repulsive Hubbard interactions are studied within a model for a time-reversal-breaking WSM with tetragonal symmetry, where we can approach the limit of weakly coupled planes and coupled chains by varying the hopping amplitudes. Using a slab geometry, we employ the variational cluster approach to describe the evolution of WSM Fermi arc surface states as a function of interaction strength. We find spin and charge density wave instabilities which can gap out Weyl nodes. We identify scenarios where the bulk Weyl nodes are gapped while the Fermi arcs still persist, hence realizing a quantum anomalous Hall state.

TT 49.3 Wed 15:30 HSZ 204

Experimental observation of type-II Weyl states in $TaIrTe_4$ — •Erik Haubold[1], Klaus Koepernik[1], Dmitriy Efremov[1], Seunghyun Khim[2], Alexander Fedorov[1,3], Yevhen Kushnirenko[1], Jeroen van den Brink[1,4], Sabine Wurmehl[1,4], Bernd Büchner[1,4], Timur Kim[5], Moritz Hoesch[5], Kazuki Sumida[6], Kazuaki Taguchi[6], Tomoki Yoshikawa[6], Akio Kimura[6], Taichi Okuda[7], and Sergey Borisenko[1] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]MPI CPfS, 01187 Dresden, Germany — [3]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany — [4]Department of Physics, TU Dresden, 01062 Dresden, Germany — [5]Diamond Light Source, Didcot OX11 0DE, United Kingdom — [6]Graduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan — [7]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

Weyl semimetals have raised a lot of interest lately due to their interesting exotic surface states. $TaIrTe_4$, belonging to the recently introduced class of type-II Weyl semimetals, hosts 4 Weyl points. These are well separated in the Brillouin zone and connected by rather long and parralel Fermi Arcs, making the material especially interesting for further research and future applications. In this work we find direct correspondence between theoretical predictions and ARPES results for both bulk and the surface states. Remarkably, these surface states are spin polarized, highlighting the potential for novel applications.

TT 49.4 Wed 15:45 HSZ 204

Magneto-optical infrared studies of the Weyl semimetals TaAs, TaP and NbP — D. Neubauer[1], R. Kemmler[1], W. Li[1], R. Hübner[2], A. Löhle[1], M. Schilling[1], M. Schmidt[3], C. Shekhar[3], C. Felser[3], M. Dressel[1], and •A. V. Pronin[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]FMQ, Universität Stuttgart, Germany — [3]MPI CPfS, Dresden, Germany

We have investigated the infrared response of TaAs, TaP, and NbP in zero magnetic field and in fields of up to 30 T. Additionally, magneto-transport measurements have been conducted on the same samples. In all compounds, we can reliably trace the transitions between different Landau levels. The transition frequencies demonstrate a square-root field dependence, typical for the linearly dispersed bands. In TaP, we can also see a sizeable shifting of the plasma edge in magnetic field and an interplay between this plasma-edge shift and the Landau-level transitions. We compare the optical spectra of the three compounds, describe the spectra by the recent models for the (magneto)-optical response of Weyl semimetals, and extract such parameters as the Fermi velocities of the carriers in the Weyl bands and the positions of the Fermi levels relative to the Weyl points.

TT 49.5 Wed 16:00 HSZ 204

Emergent Weyl fermion bulk excitations in TaP evidenced from ^{181}Ta quadrupole resonance — H. Yasuoka[1,2], T. Kubo[1,3], Y. Kishimoto[1,3], D. Kasinathan[1], M. Schmidt[1], B. Yan[1], Y. Zhang[4], H. Tou[3], C. Felser[1], A.P. Mackenzie[1,5], and •M. Baenitz[1] — [1]MPI for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Japan — [3]Department of Physics, Graduate school of Science, Kobe University, Kobe, Japan — [4]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [5]SUPA, School of Physics & Astronomy, University of St. Andrews, UK

The monophosphite TaP has a non centrosymmetric structure and sizable spin orbit coupling and belongs the class of Weyl semimetals. A crossing of lineare dispersive ($E \propto k$) topologically protected polarized bands in a single point in reciprocal space defines the Weyl node where the fermion mass vanishes theoretically and a giant orbital hyperfine coupling is expected [1]. ^{181}Ta quadrupole resonance (NQR) resolves three NQR lines associated to the split level transitions for I=7/2 Ta. The spin lattice relaxation was measured for the $\pm 5/2 \leftrightarrow \pm 3/2$ transition. Above 30 K, a pronounced $(1/T_1T) \propto T^2$ is found. We attributed this to the magnetic excitations of Weyl fermions ($N(E) \propto E^2$) with temperature dependent orbital hyperfine coupling in agreement with the prediction from theory [1].

[1] Z. Okvatovity et al., arXiv:1609.3370v1

15 min. break.

TT 49.6 Wed 16:30 HSZ 204

Magnetic Properties of Dirac Fermions in a Family of Anti-perovskites — •Moritz Mandes Hirschmann and Andreas Philipp Schnyder — Max Planck Institute for Solid State Research, Stuttgart, Germany

We study the magnetic properties of the anti-perovskite materials A_3EO, where A denotes an alkaline earth metal, while E stands for Pb or Sn. The low-energy electronic properties of this family of anti-perovskites is described by three-dimensional Dirac fermions, which are gapped out by spin-orbit coupling [1-3]. We discuss the magnetic response of this Dirac electron system, considering both orbital and spin Zeeman effects. Interestingly, a strong Zeeman field splits the gapped Dirac cones into ungapped Weyl points, which are protected by a quantized Chern number. The compound Eu_3PbO breaks in its ferromagnetic phase intrinsically the time-reversal symmetry by exhibiting a magnetization that corresponds to a large Zeeman splitting at the Europium atoms. Again we observe Weyl points in the band structure. Using a tight-binding description we calculate these Chern numbers and demonstrate that the Weyl points are connected by Fermi arcs in the surface Brillouin zone. Furthermore, we determine the Landau level structure of the gapped Dirac electrons.

[1] T. H. Hsieh, J. Liu, and L. Fu. *Phys. Rev. B*, 90:081112, Aug 2014
[2] J. Nuss, C. Mühle, K. Hayama, V. Abdolazimi, and H. Takagi. *Acta Crystallographica Section B*, 71(3):300-312, Jun 2015.
[3] D. Samal, H. Nakamura, and H. Takagi. *APL Mater.*, 4(7), 2016.

TT 49.7 Wed 16:45 HSZ 204

Emergent Weyl points from Floquet Weyl semimetals in the resonant limit — •Leda Bucciantini[1], Stithadi Roy[1], Sota Kitamura[2], and Takashi Oka[1] — [1]Max Planck Institute for Physics of Complex Systems, Germany — [2]Tokyo University, Japan

We investigate the formation of Weyl points from a Dirac semimetal after shining it with circularly polarized light, focusing on the resonant frequency limit. Within a Floquet formalism, we describe the phase

diagram as a function of the intensity and frequency of the laser. A couple of Weyl points split both from the original Dirac point and from the Floquet side bands. Increasing the value of the laser intensity, the Weyl points emerging from the original Dirac point and the side band merge, annihilate and then gap out. We also compute the monopole charge for each of the emergent Weyl points.

TT 49.8 Wed 17:00 HSZ 204

Self-forming superconducting microstructures from Weyl semi-metals — •Maja D. Bachmann[1], Nityan Nair[3], Felix Flicker[3], Roni Ilan[3], Nirmal J. Ghimire[2], Eric D. Bauer[2], Filip Ronning[2], James G. Analytis[3], and Philip J.W. Moll[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Los Alamos National Laboratory, Los Alamos, NM, USA — [3]Department of Physics, University of California Berkeley, CA, USA

The non-trivial topology of the bulk bands in topological semi-metals protects new electronic states at the surface, such as the famous Fermi arc states. If a superconducting gap is induced in these materials, exotic electronic states are expected to appear at the interface such as zero-energy Majorana modes. These novel states provide insights into the topological aspects of electronic matter and are of interest for quantum coherent applications. Here we will present a new route to reliably fabricating superconducting microstructures from the intrinsically non-superconducting Weyl semi-metals NbAs and TaAs under ion irradiation. The large difference in the surface binding energy of Nb/Ta and As leads to a natural enrichment of Nb/Ta at the surface during ion milling, forming a superconducting surface layer (Tc~3.5K). Being formed from the target crystal itself, the ideal contact between the superconductor and the bulk enables an effective gapping of the nodes due to the proximity effect. Simple low energy ion irradiation may thus serve as a powerful tool to fabricate topological quantum devices from mono-arsenides, even on an industrial scale.

TT 49.9 Wed 17:15 HSZ 204

Angle-dependent magnetoresistance in Weyl semimetals with long-range disorder — •Jan Behrends[1] and Jens H Bardarson[1,2] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]Department of Theoretical Physics, KTH Royal Institute of Technology, Stockholm, SE-106 91 Sweden

The chiral anomaly is one of the most intriguing features of Weyl semimetals. It states that left- and right-handed fermions are not conserved individually, while their sum is. One of its experimental consequences is the negative magnetoresistance predicted in Weyl semimetals. Recent experiments show strong indications for such an anomalous conductivity response, while some outstanding issues remain. Most prominently, the anomalous response is much more sharply peaked for parallel magnetic and electric fields than expected from simple theoretical considerations. Here, we investigate scattering in Weyl semimetals in presence of magnetic fields for a correlated disorder potential. We find a decrease of the internode relaxation time when the magnetic field is tilted away from the separation of the Weyl nodes. Since the internode relaxation time is proportional to the anomaly-related conductivity, this feature may explain the narrow current plume seen experimentally.

TT 49.10 Wed 17:30 HSZ 204

Surface states in holographic Weyl semimetals — •Markus Heinrich, Amadeo Jimenez-Alba, Sebastian Möckel, and Martin Ammon — Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena

Weyl semimetals (WSMs) are a class of gapless topological materials with low-energy excitations behaving as Weyl fermions. Their most prominent feature are topologically protected surface states, so-called Fermi arcs, which were recently tied to an effective axial magnetic field arising at a surface due to lattice deformations. As in the chiral magnetic effect, this field gives rise to an anomalous current at finite chemical potential which is localised at the surface. We performed its subtle computation in the strong coupling limit by using a holographic model. We found a non-trivial unversality of the current, allowing us to interpret it in a simple Fermi arc-like picture. In the end, I will discuss the limits of this universality.

TT 50: Correlated Electrons: Frustrated Magnets - Low-Dimensional Systems

Time: Wednesday 15:00–18:00 Location: HSZ 304

TT 50.1 Wed 15:00 HSZ 304

Quantum Monte Carlo simulations of a frustrated ladder in the dimer basis — •Andreas Honecker[1] and Stefan Wessel[2] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, Université de Cergy-Pontoise, France — [2]Institut für Theoretische Festkörperphysik, RWTH Aachen University, Germany

Frustrated quantum spin systems are notorious for the infamous "sign problem" that prohibits efficient Quantum Monte Carlo simulations in relevant temperature regions. However, the sign problem is basis dependent. Indeed, recent works [1,2] have shown that passing to a rung-dimer basis eliminates the sign problem for the case of a highly frustrated two-leg spin-1/2 ladder where diagonal couplings are equal to the leg couplings. Here we generalise this result to the case where the two couplings along the legs remain antiferromagnetic but are in general different. We find that although the sign problem re-appears in general, it remains sufficiently mild throughout the phase diagram of the frustrated ladder such that efficient Quantum Monte Carlo simulations can be performed, yielding accurate results for thermodynamic quantities such as magnetic susceptibility and specific heat.

[1] A. Honecker, S. Wessel, R. Kerkdyk, T. Pruschke, F. Mila, B. Normand, Phys. Rev. B **93** (2016) 054408
[2] F. Alet, K. Damle, S. Pujari, Phys. Rev. Lett. **117** (2016) 197203

TT 50.2 Wed 15:15 HSZ 304

Effective spin-Hamiltonian for the 1D Hubbard model at arbitrary coupling strength — Rolf Schumann[1] and •Stefan-Ludwig Drechsler[2] — [1]Institut für Theoretische Physik, TU Dresden, D-01062,Germany — [2]Institute for Solid State Theory, Leibniz-Instiitute IFW-Dresden, D-01171 Dresden. Germany

Using exact diagonalization analytical results for small clusters (dimers, trimers and tetramers) we derive an approximate *effective* spin-Hamiltonian valid for any ratio $u = U/t$, where U denotes the on-site Coulomb repulsion and t is the nearest neighbor (NN)-transfer integral. Thereby we present analytical results for the first, second (NNN), third neighbor exchange integrals $J_1 \gg J_2 \gg J_3$, respectively, and also for the leading cyclic quartic (four spin) exchange term. All interaction parameters are smooth monotonous functions of u without any artificial divergency at $u = 4$ or even $u = 0$ as in other methods based on perturbational theory. Our results compare well with those for the NN (analytical expression) and the NNN (numerical data are available in the limit $u \geq 4$, only) exchange integrals J_1 and J_2, respectively, obtained within the flow-equation technique [1,2]. Possible applications for "conducting" polymers and spin-Peierls systems being in the intermediate coupling regime are briefly disussed.

[1] S.A. Hamerla *et al.*, Phys. Rev. B **82**, 235117 (2010)
[2] S.A. Hamerla and G. Uhrig, unpublished.

TT 50.3 Wed 15:30 HSZ 304

Ground-state phase diagram of the $J_1 - J_1' - J_2$ chain — •Clió Efthimia Agrapidis[1,2], Stefan-Ludwig Drechsler[1], Jeroen van den Brink[1,2], and Satoshi Nishimoto[1,2] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany — [2]Department of Physics, Technical University, Dresden, 01069 Dresden, Germany

Quasi one-dimensional (1D) frustrated systems, despite their simple structure, are at the center of attention as a playground for novel ground states that can emerge from frustration and strong quantum fluctuations due to low dimensionality. Motivated by the extensive interest in this field and by recent experimental results, we study the one-dimensional Heisenberg model with dimerized nearest-neighbor ferromagnetic ($J_1, J_1' < 0$) and next-nearest-neighbor antiferromagnetic ($J_2 > 0$) couplings using the spin-wave theory and the density-matrix renormalization group technique. Based on the numerical calculations of total spin, spin gap, equal-time spin-spin correlation functions, and Tomonaga-Luttinger spin exponent, we present the ground-state phase

diagram in the space of frustration ratio ($\alpha = J_2/|J_1|$) and dimerization degree ($\beta = J_1'/J_1$). We find a first-order transition between fully-polarized FM and incommensurate singlet state at $\alpha_c = (\beta/2)/(1+\beta)$ and we suggest the existence of a crossover between an AKLT-type valence bond solid state and a frustration-induced dimerized state in the gapped phase. In the absence of dimerization ($\beta = 1$), the spin gap opens at $1/4 < \alpha \lesssim 1.52$. Relevance to the quasi-one-dimensional frustrated compounds $LiCuSbO_4$ and $Rb_2Cu_2Mo_3O_{12}$ is also discussed.

TT 50.4 Wed 15:45 HSZ 304

Dynamic structure factor of disordered quantum spin ladders — •Max Hörmann and Kai Phillip Schmidt — Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

We investigate the zero-temperature dynamic structure factor of a two-leg spin-1/2 Heisenberg ladder with quenched disorder relevant for inelastic neutron scattering. To this end we apply perturbative continuous unitary transformations about the limit of isolated rungs using a white-graph expansion [1] to derive the physical properties of the elementary triplon excitations of the disordered spin ladder in the thermodynamic limit. Here we study bimodal disorder on rungs and legs realizable in experiments by intential doping of existing spin-ladder compounds. We focus on the one-triplon properties which we calculate with high precision in the weakly-coupled rung regime. We observe that the dynamic structure factor displays characteristic differences in rung and leg disorder.

[1] K. Coester and K.P. Schmidt, Phys. Rev. E 92, 022118 (2015).

TT 50.5 Wed 16:00 HSZ 304

Critical behavior of quantum magnets with long-range interactions in the thermodynamic limit — •Sebastian Fey — Lehrstuhl für Theoretische Physik I, Staudtstraße 7, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Quasi-particle properties of quantum magnets with long-range interactions are investigated by high-order linked-cluster expansions in the thermodynamic limit. It is established that perturbative continuous unitary transformations on white graphs are a promising and flexible approach to treat long-range interactions in quantum many-body systems. We exemplify this scheme for the one-dimensional transverse-field Ising chain with long-range interactions. For this model the elementary quasi-particle gap is determined allowing to access the quantum-critical regime including critical exponents and multiplicative logarithmic corrections for the ferro- and antiferromagnetic case.

TT 50.6 Wed 16:15 HSZ 304

The dynamics of linarite: Observations of magnetic excitations — Kirrily C. Rule[1], Britta Willenberg[2,3], Markus Schäpers[4], Anja U.B. Wolter[4], Stefan L. Drechsler[4], Georg Ehlers[5], Alan Tennant[5], Richard Mole[1], Jason Gardner[6,7], •Stefan Süllow[2], and Satoshi Nishimoto[4,8] — [1]ANSTO, Kirrawee, Australia — [2]IPKM, TU Braunschweig, Braunschweig, Germany — [3]HZB für Materialien und Energie, Berlin, Germany — [4]IFW Dresden, Dresden, Germany — [5]ORNL, Oak Ridge, USA — [6]NSRRC, Hsinchu, Taiwan — [7]CCMS, National Taiwan University, Taipei, Taiwan — [8]Dept. Physics, TU Dresden, Dresden, Germany

Here we present inelastic neutron scattering measurements from the frustrated, quantum spin-1/2 chain material linarite, $PbCuSO_4(OH)_2$. Time of flight data, taken at 0.5 K and zero applied magnetic field reveals low-energy dispersive spin wave excitations below 1.5 meV both parallel and perpendicular to the Cu-chain direction. From this we confirm that the interchain couplings within linarite are around 10 % of the nearest neighbour intrachain interactions. We analyse the data within both linear spin-wave theory and density matrix renormalisation group theories and establish the main magnetic exchange interactions and the simplest realistic Hamiltonian for this material.

15 min. break.

TT 50.7 Wed 16:45 HSZ 304

DMRG simulations of SU(N) Heisenberg models using a million of states — •Andreas Weichselbaum[1], Sylvain Capponi[2], Andreas Läuchli[3], Alexei Tsvelik[4], and Philippe Lecheminant[5] — [1]Ludwig Maximilians University, Munich, Germany — [2]CNRS Toulouse, Université Paul Sabatier, France — [3]University of Innsbruck, Austria — [4]Brookhaven National Laboratory, Upton, NY, USA — [5]Université de Cergy Pontoise, France

The density matrix renormalization group (DMRG) is applied to SU(N) symmetric Heisenberg chains and ladders while fully exploiting the underlying SU(N) symmetry. Since these models can be motivated from symmetric N-band fermionic models, it is immediately clear that the numerical complexity of simulating SU(N) symmetric models grows exponentially in N. Nevertheless in the presence of symmetry this exponential growth is largely transferred to the symmetry multiplets in that the largest multiplets that appear in a typical simulation grow exponentially in size like 10^{N-1}. Therefore while keeping a moderate number of multiplets, the full state space dimension required for converged results can quickly reach a million of states. Recent results on Heisenberg ladders with $N \leq 5$ and varying rung coupling are discussed and contrasted to existing literature.

TT 50.8 Wed 17:00 HSZ 304

Unconventional nematic state in the frustrated and anisotropic spin-chain cuprate $LiCuSbO_4$ — •Satoshi Nishimoto[1,2], Hans-Joachim Grafe[1], Margarita Iakovleva[1,3], Evgeniia Vavilova[1,3], Alexey Alfonsov[1], Mihai-I. Sturza[1], Helge Rosner[4], Johannes Richter[5], Ulrich Rössler[1], Stefan-Ludwig Drechsler[1], Vladislav Kataev[1], and Bernd Büchner[1,2] — [1]IFW Dresden, Germany — [2]TU Dresden, Germany — [3]Zavoisky Physical Technical Institute, Kazan, Russia — [4]MPI-cPfS, Dresden, Germany — [5]U. Magdeburg, Germany

Modern theories of quantum magnetism predict exotic multipolar states in frustrated spin-1/2 Heisenberg chains with ferromagnetic nearest-neighbor (NN) inchain exchange in high magnetic fields. Experimentally these states remained elusive so far. Here we report the evidence for a long-sought magnetic field-induced nematic state arising above a field of ~ 13 T in the edge-sharing chain cuprate $LiCuSbO_4$. This interpretation is based on the observation of a field induced spin-gap in the measurements of the ^{7}Li NMR spin relaxation rate T_1^{-1} as well as a contrasting field-dependent power-law behavior of T_1^{-1} vs. T and is further supported by static magnetization and ESR data. An underlying theoretical microscopic approach favoring a unconventional nematic scenario is based essentially on the NN XYZ exchange anisotropy within a model for frustrated spin-1/2 chains. It is investigated by the DMRG technique. The employed exchange parameters are justified qualitatively by electronic structure calculations for $LiCuSbO_4$.

TT 50.9 Wed 17:15 HSZ 304

Structural and Magnetic Properties of the trirutile-type 1D Heisenberg Antiferromagnet $CuTa_2O_6$ — •Aleksandr Golubev[1], R. E. Dinnebier[1], A. Schulz[1], R. K. Kremer[1], H. Langbein[2], A. Senyshyn[3], J. M. Law[4], Th. Hansen[5], E. E. Gordon[6], and M.-H. Whangbo[6] — [1]MPI for Solid State Research, D-70569 Stuttgart, Germany — [2]Institut für Anorganische Chemie der TUD, D-01062 Dresden, Germany — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), TUM, D-85747 Garching, Germany — [4]Dresden High Magnetic Field Laboratory (HLD), D-01314 Dresden-Rossendorf, Germany — [5]ILL, B.P. 156, 38043 Grenoble, France — [6]Department of Chemistry, NCSU, Raleigh, North Carolina 27695-8204, USA

Polycrystalline samples of $CuTa_2O_6$ prepared by low-temperature decomposition of Cu-Ta-oxalate precursors at room temperature crystallize with a monoclinically distorted trirutile structure type. By detailed high temperature x-ray and neutron powder diffraction studies we detected a structural phase transition to the tetragonal trirutile structure-type at 503(3) K. The structural phase transition was ascertained by Raman scattering. GGA+U DFT calculations of the spin exchange parameters, magnetic susceptibility and isothermal magnetization measurements constitute $CuTa_2O_6$ as new 1D Heisenberg chain with predominant afm nearest neighbor exchange interaction $J_{nn} \approx 50$ K. Heat capacity and low temperature high intensity neutron powder diffraction studies could not find long range order down to 0.4K.

TT 50.10 Wed 17:30 HSZ 304

Intertwined nematic orders in a frustrated ferromagnet — •Yasir Iqbal[1], Pratyay Ghosh[2], Rajesh Narayanan[3], Brijesh Kumar[2], Johannes Reuther[4,5], and Ronny Thomale[1] — [1]Institute for Theoretical Physics, Universität Würzburg, 97074 Würzburg, Germany — [2]Jawaharlal Nehru University, New Delhi 110067, India — [3]Indian Institute of Technology Madras, Chennai 600036, India — [4]Freie Universität Berlin, 14195 Berlin, Germany — [5]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

We investigate the quantum phases of the frustrated spin-$\frac{1}{2}$ J_1-J_2-

J_3 Heisenberg model on the square lattice with ferromagnetic J_1 and antiferromagnetic J_2 and J_3 interactions. Using the pseudo-fermion functional renormalization group technique, we find an intermediate paramagnetic phase located between classically ordered ferromagnetic, stripy antiferromagnetic, and incommensurate spiral phases. We observe that quantum fluctuations lead to significant shifts of the spiral pitch angles compared to the classical limit. By computing the response of the system with respect to various spin rotation and lattice symmetry-breaking perturbations, we identify a complex interplay between different nematic spin states in the paramagnetic phase. While retaining time-reversal invariance, these phases either break spin-rotation symmetry, lattice-rotation symmetry, or a combination of both. We therefore propose the J_1-J_2-J_3 Heisenberg model on the square lattice as a paradigmatic example where different intimately connected types of nematicities emerge in the same model.

TT 50.11 Wed 17:45 HSZ 304

Topological quantum paramagnet in a quantum spin ladder — •Darshan G. Joshi and Andreas P. Schnyder — Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany

Recently, it has been shown that analogs of quantum Hall systems could be realized in quantum magnets. Most of these works have focused on the symmetry broken phases in magnetic systems. In this work, we consider the dimer-quantum-paramagnetic phase of a S=1/2 quantum spin ladder, which does not break any symmetry of the parent Hamiltonian. We show that in the presence of Dzyaloshinskii-Moriya interaction and external magnetic field the paramagnetic phase is actually split into a topologically trivial and a topologically non-trivial phase. We calculate the winding number and the end-states in this topologically non-trivial phase. The topological aspect is a consequence of the reflection symmetries present in the model and other models with similar properties may also realize the same physics.

TT 51: Topological Insulators (joint session DS, HL, MA, O, TT, organized by MA)

Time: Wednesday 15:00–18:00 Location: HSZ 401

TT 51.1 Wed 15:00 HSZ 401

Mn-doped topological insulators Bi_2Te_3 and Bi_2Se_3: an ab initio study of magnetism and transport properties — •Karel Carva[1], Pavel Baláž[1], Jakub Šebesta[1], Josef Kudrnovský[2], František Máca[2], and Václav Drchal[2] — [1]Charles University, DCMP, Ke Karlovu 5, CZ-12116 Prague, Czech Republic — [2]Institute of Physics, ASCR,Na Slovance 2, CZ-18221 Prague, Czech Republic

For the interpretation of experiments studying the Bi_2Te_3 and Bi_2Se_3 family of topological insulators it is necessary to include the native defects into the picture. Using similar methods one can study also the magnetic doping, which has attracted a lot of interest recently [1]. We calculate on an ab initio level the electronic structure of Bi_2Te_3 and Bi_2Se_3 doped by Mn at different possible positions and also in the presence of native antisites and vacancies. This provides for the first time a comprehensive map of possible behavior affecting strongly the bulk resistivity, carrier concentration and magnetism. It allows us to tune these properties, and also help to uncover the location of Mn atoms, since the substitutional or interstitial Mn placement exhibits strikingly different properties. Calculations indicate that the presence of interstitials may help to understand experimental observations[2].

Exchange interactions between Mn magnetic moments in bulk Mn-doped Bi_2Te_3 / Bi_2Se_3 have been calculated using ab initio methods. These results allow us to study the Curie temperatures by means of atomistic Monte Carlo simulations.

[1] Y. S. Hor et al., Phys. Rev. B 81, 195203 (2010)
[2] K. Carva et al., Phys. Rev. B 93, 214409 (2016)

TT 51.2 Wed 15:15 HSZ 401

Unraveling the Spin Structure of Unoccupied States in Bi_2Se_3 — •Christian Langenkämper[1], Anna Zumbülte[1], Jürgen Braun[2], Tobias Förster[3], Anke B. Schmidt[1], Jianli Mi[4], Bo Iversen[4], Philip Hofmann[5], Jan Minár[2,6], Hubert Ebert[2], Peter Krüger[3], Michael Rohlfing[3], and Markus Donath[1] — [1]Physikalisches Institut, WWU Münster, Germany — [2]Department of Chemistry, LMU München, Germany — [3]Institut für Festkörpertheorie, WWU Münster, Germany — [4]Center for Materials Crystallography, Department of Chemistry, Aarhus University, Denmark — [5]Department of Physics and Astronnomy, Interdisciplinary Nanoscience Center, Aarhus University, Denmark — [6]New Technologies Research Centre, University of West Bohemia Pilzen, Czech Republic

The control of spin currents in topological insulators using optical transitions opens new perspectives in (opto-)spintronics. To understand these processes involving topological surface states, a profound knowledge about the dispersion and the spin polarization of both the occupied and the unoccupied electronic states is crucial. We present a joint experimental and theoretical study on the unoccupied electronic states of Bi_2Se_3. We discuss spin- and angle-resolved inverse photoemission results in comparison with calculations for both the intrinsic band structure and, within the one-step model of (inverse) photoemission, the expected spectral intensities. This allows us to unravel the intrinsic spin texture of the unoccupied bands at the surface of Bi_2Se_3.

TT 51.3 Wed 15:30 HSZ 401

Enhanced Mobility of Spin-Helical Dirac Fermions in Disordered 3D Topological Insulators — Joseph Dufouleur[1], Louis Veyrat[1], Bastien Dassonneville[1], Christian Nowka[1], Silke Hampel[1], Pavel Leksin[1], Barbara Eichler[1], Oliver G. Schmidt[1], Bernd Büchner[1], and •Romain Giraud[1,2] — [1]IFW, Dresden, Germany — [2]INAC-SPINTEC, Grenoble, France

We reveal the enhanced transport length of 2D spin-helical Dirac fermions in highly-disordered 3D topological insulators, due to anisotropic scattering, by electrical transport measurements of Bi_2Se_3 nanostructures [1]. By comparing the quantum mobility, related to the electronic mean-free path, to the mobility obtained from transconductance measurements, related to the transport length (backscattering), we evidence the long-range nature of the scattering potential for surface Dirac fermions and some limitation due to a residual bulk/surface coupling. In wide nanostructures, it is shown that the long phase coherence length results from the enhanced diffusion constant, in very good agreement with results obtained from previous studies of the weak anti-localization [2]. Our work suggests that the spin-flip length ($l_{sf} \approx l_{tr}$) could reach the micron size in materials with a reduced bulk doping, which reveals the true potential for building functionalized spintronic and ballistic electronic devices out of disordered 3D topological insulators.

[1] J. Dufouleur et al., Nano Lett. 16, 6733 (2016)
[2] Z. Li et al., Phys. Rev. B 91, 041401 (2015)

TT 51.4 Wed 15:45 HSZ 401

Spin-dependent very-low-energy electron diffraction at Bi_2Se_3 — •Andre Reimann[1], Christian Langenkämper[1], Anna Blob[1], Jürgen Braun[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Department Chemie, Ludwig-Maximilians-Universität München, Germany

The topological insulator Bi_2Se_3 exhibits prominent spin effects in both the occupied and unoccupied electronic bandstructure due to strong spin-orbit coupling. This promises large effects also for spin-dependent electron reflection.

We present a combined experimental and theoretical study of the spin-dependent electron reflection of Bi_2Se_3 along the $\overline{\Gamma}\,\overline{K}$ and the $\overline{\Gamma}\,\overline{M}$ direction. Experimentally we performed spin-dependent very-low-energy electron diffraction (VLEED) experiments over a wide range of energies and angles of incidence. Theoretically we used ab-initio calculations by means of the SPKKR layer code.

For both directions, we derived maps for the reflectivity and the Sherman function. We found high spin asymmetries up to 37%, which are caused by the large spin-orbit coupling of Bi_2Se_3. These features show a strong energy and angle dependence. Futhermore, we identified the VLEED finestructures, which contain information about the surface barrier.

TT 51.5 Wed 16:00 HSZ 401

Theoretical investigations of magnetically doped topological insulators — •Jan Minar[1,2], Jürgen Braun[1], Hubert Ebert[1],

Jaime Sanchez-Barriga[3], Oliver Rader[3], Jan Honolka[4], and Andreas Ney[5] — [1]LMU München, Germany — [2]University of West Bohemia, Plzen, Czech Rep. — [3]Helmholz Zentrum, Berlin — [4]ASCR, Institute of Physics, Prague — [5]Johannes Kepler University Linz, Austria

Band gap opening of topological surface states due to magnetic doping is the subject of a long standing and ongoing discussion. However, in spite of the progress made during the last years in this field there are still phenomena that are poorly understood and many open issues to be addressed. In several cases, like for example Mn doped Bi_2Se_3 band gap opening does not seem to be of magnetic origin. We will present several examples for detailed theoretical studies on various bulk as well as surface doped topological insulators performed by means of the SPR-KKR band structure method. Our results will be discussed in direct comparison with corresponding ARPES [1], XAS and XMCD [2,3] experimental data.

[1] J. Sanchez-Barriga et al., Nat. Communications, 7, 10559 (2016)
[2] A. Ney et al., in preparation
[3] J. Honolka et al., PhysRevB 94, 161114 (2016)

15 min. break.

TT 51.6 Wed 16:30 HSZ 401

Lifetime and surface to bulk scattering of the topological surface state in 3D topological Insulators — •Philipp Rüssmann, Phivos Mavropoulos, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Doping of topological insulators, such as Bi_2Se_3 or Bi_2Te_3, may result in a shift of the Fermi level to a position where the Topological Surface States (TSS) and the bulk states coexist. Then, the TSS lifetime τ_s due to impurity scattering is decomposed in surface-to-surface and surface-to-bulk contributions with scattering rates τ_{ss}^{-1} and τ_{sb}^{-1}, respectively, where $\tau_s^{-1} = \tau_{ss}^{-1} + \tau_{sb}^{-1}$. We investigate this decomposition in Bi_2Se_3 and Bi_2Te_3 by means of density-functional calculations.

In a detailed analysis we find that conduction and valence band play a different role in the surface to bulk state scattering. Especially for the important case of n-doping, the conduction band contribution is very small compared to the surface-state contribution. As a consequence, the surface electrons remain topologically protected in spite of coexisting bulk bands.

For the calculation of electronic structure and scattering properties we employed the full potential relativistic Korringa-Kohn-Rostoker Green-function method. 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.

TT 51.7 Wed 16:45 HSZ 401

Surfaces and interfaces of topological insulators from relativistic many-body calculations. — •Irene Aguilera, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany.

We present a description of surfaces of topological insulators (TIs) as well as interfaces between different TIs and between TIs and trivial materials. We focus on materials of the Bi_2Se_3 family. We use the all-electron FLAPW formalism and the relativistic many-body *GW* method [1]. Including many-body effects in the calculation and incorporating the spin-orbit coupling into the self-energy are critical to obtain reliable results for these TIs [1-5]. For the description of surface and interface states, we use a basis of Wannier functions to construct the slabs and heterostructures Hamiltonians. This approach allows us to study very large systems with a high accuracy. We discuss the differences between surface and interface states and the interaction ("crosstalk") between energetically non-degenerate Dirac cones at the interface and surfaces of the heterostructure.

[1] Aguilera *et al.*, Phys. Rev. B **88**, 165136 (2013). [2] Aguilera *et al.*, Phys. Rev. B **91**, 125129 (2015). [3] Aguilera *et al.*, Phys. Rev. B **88**, 045206 (2013). [4] Nechaev *et al.*, Phys. Rev. B **87**, 121111(R) (2013). [5] Michiardi *et al.*, Phys. Rev. B **90**, 075105 (2014).

Financial support from the Virtual Institute for Topological Insulators of the Helmholtz Association.

Correspondence: i.aguilera@fz-juelich.de

TT 51.8 Wed 17:00 HSZ 401

Topological thin films of Bi and InBi coexisting on InAs(111) — •L Nicolai[1,2,7], K Hricovini[1,2], J-M Mariot[1,3], M C Richter[1,2], O Heckmann[1,2], U Djukic[1], T Balasubramanian[4], M Leandersson[4], J Sadowski[4], J Denlinger[5], I Vobornik[6], J Braun[7], H Ebert[7], and J Minar[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 Munich, Germany — [8]Univ. of West Bohemia, Plzeñ, Czech Rep.

The Bi(111) surface is a prototype system that shows 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 behavior was suggested for a variable film thickness as a function of the layer thickness [2]. This clearly indicates that the electronic properties of thin films of this material are quite complex and far from being fully understood. Here we present combined theoretical and ARPES studies on the electronic structure of Bi(111) films grown on InAs(111). Bi grows epitaxially on this substrate and a monocrystal of very high quality is obtained after depositing several monolayers. ARPES experiments on the samples prepared show several new electronic states not reported before. The one-step model of photoemission as implemented in the SPR-KKR package [3] allows us to identify pristine Bi bulk states coexisting with InBi surface states. [1] Wada et *al.*, Phys. Rev. B 83,121310 (2011) [2] Liu et *al.*, Phys. Rev. Lett. 107, 136805 (2011) [3] Braun, Rep. Prog. Phys. 59, 1267-1338 (1996)

TT 51.9 Wed 17:15 HSZ 401

Instability of the topologically protected surface state in Bi_2Se_3 upon deposition of gold — •Andrey Polyakov[1], Holger L. Meyerheim[1], Christian Tusche[2], Daryl E. Crozier[3], and Arthur Ernst[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany, Germany — [3]Department of Physics, Simon Fraser University Burnaby, BC Canada, V5A 1S6

We present an experimental and theoretical analysis of the stability of the Topological surface state (TSS) in Bi_2Se_3 upon sub-monolayer deposition of Au. Extended x-ray absorption fine structure experiments provide clear evidence that Au -when deposited on the (0001) surface kept at 160 K- substitutes Bi atoms within the first quintuple layer. This goes in parallel with the dramatic weakening of the spectral density of the TSS as observed by angular resolved photoemission. In accordance with first-principles calculations, Au in Bi substitutional sites within the first QL creates a d-type resonant state near E_F, which hybridizes with the TI bands and substantially modifies its surface electronic structure. According to the model of Black-Schaffer et al. [1] a bulk-surface interaction is a prerequisite for the gap opening, since the TSS is not protected by scattering processes involving bulk three-dimensional states. References: [1] A. M. Black-Schaffer and A. V. Balatsky, Phys. Rev. B 86, 115433 (2012). Acknowledgements: Work supported by SPP 1666. Work at the APS is supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

TT 51.10 Wed 17:30 HSZ 401

Magnetic exchange on the surface of topological insulators — •Alessandro Barla[1], Sanjoy K. Mahatha[1], Paolo Sessi[2], Kai Fauth[2], Thomas Bathon[2], Matthias Bode[2], Miguel Angel Valbuena[3], Sylvie Godey[3], Aitor Mugarza[3], Pierluigi Gargiani[4], Philipp Rüssmann[5], Phivos Mavropoulos[5], Gustav Bihlmayer[5], Stefan Blügel[5], and Carlo Carbone[1] — [1]Istituto di Struttura della Materia, CNR, I-34149 Trieste, Italy — [2]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, D-97074 Würzburg, Germany — [3]Catalan Institute of Nanoscience and Nanotechnology (ICN2), E-08193 Cerdanyola del Vallès, Spain — [4]ALBA Synchrotron Light Source, E-08290 Cerdanyola del Vallès, Spain — [5]PGI-1 and IAS-1, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Three-dimensional topological insulators have conducting surface states in the bulk band gap, protected by time-reversal symmetry, which locks spin with momentum. It was shown, however, that surface magnetic doping can break time-reversal symmetry and induces backscattering of Dirac states [1]. We present the results of our investigations of the magnetic properties of individual atoms of 3d transition metals (Mn, Fe, Co) deposited on the surface of the topological insulator Bi_2Te_3. All studied adatoms present an out-of-plane magnetic anisotropy associated with sizeable orbital moments and we find evidence of surface-mediated magnetic exchange interactions which are

of opposite sign for Mn and Co.
[1] P. Sessi et al., Nat. Commun. 5, 5349 (2014).

15 min. break.

TT 52: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - V (joint session DS, HL, MA, MM, O, TT, organized by O)

Time: Wednesday 15:00–18:15 Location: GER 38

TT 52.1 Wed 15:00 GER 38

First-principle Linear Response in Real Space — •Honghui Shang[1], Danilo S. Brambila[1], Christian Carbogno[1], Patrick Rinke[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Aalto University, Helsinki, Finland

Density-functional perturbation theory (DFPT) has developed into an important computational tool for assessing the linear electronic response of crystalline solids to perturbations, e.g., from electric fields or nuclear displacements [1]. In this work we present a full real-space reformulation of DFPT and its implementation [2] in the all-electron, numeric atom-centered orbital electronic structure theory code FHI-aims. We discuss the specific contributions, e.g., relativistic effects and Pulay terms, that arise in such a formulation and validate our implementation by systematically comparing with the finite-difference approach for various extended systems. The computational efficiency is then analyzed via scaling and scalability tests on massively parallel architectures (CRAY and IBM x86 clusters). Finally, we show that this real-space formalism enables an arbitrarily dense sampling of the Brillouin zone by numerically cheap Fourier transformations, which in turn facilitates an efficient evaluation of the electron-phonon coupling matrix elements. We demonstrate the efficiency by computing the relaxation time of hot carriers in Si.
[1] X. Gonze and C. Lee, *Phys. Rev. B* **55**, 10355, (1997).
[2] H. Shang, *et al.*, *Comp. Phys. Comm. (accepted)*, arXiv:1610.03756.

TT 52.2 Wed 15:15 GER 38

Anharmonic Vibrations in Solids: Why and When Going Beyond Perturbative Treatments is Necessary — •Hagen-Henrik Kowalski, Maja-Olivia Lenz, Christian Carbogno, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

In *ab initio* theory, the nuclear motion is typically assessed using a truncated second order Taylor expansion for the potential energy (harmonic approximation). Recent computational and methodological advancements [1] allow to extend this expansion to the third order so to approximately treat also anharmonic effects. Little is known, however, about the role of higher order terms. In this contribution, we systematically compare how a third-order expansion performs with respect to techniques that are able to capture higher degrees of anharmonicity, e.g., the quasi-harmonic approximation and fully anharmonic molecular dynamics. For this purpose, anharmonic properties such as the thermal expansion and the Grüneisen parameters are computed for a set of materials with increasing degree of anharmonicity (Si, Mg_2Si, CuCl, and ZrO_2). This reveals that a third order expansion can still lead to quantitative and even qualitative errors at elevated temperatures and/or in highly anharmonic systems. Eventually, we discuss the impact of the chosen exchange-correlation functionals on these calculations and the implications of these findings for the computation of thermal conductivities [2].
[1] D. A. Broido, *et al.*, *Appl. Phys. Lett.* 91, 231922 (2007).
[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *ArXiv:* 1608.06917.

TT 52.3 Wed 15:30 GER 38

Anharmonic and Quantum Fluctuations in Molecular Crystals from Ab Initio Simulations — •Mariana Rossi[1] and Michele Ceriotti[2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin — [2]École Polytechnique Fédérale de Lausanne, Switzerland

Molecular crystals often exist in multiple competing polymorphs which are challenging to be predicted computationally, but show significantly different physicochemical properties. This challenge is not due only to the combinatorial search space, but also to the complex interplay of subtle effects determine the relative stability of different structures. Here we estimate all contributions to the free energies of these systems with density-functional theory, including the oft-neglected anharmonic contributions and nuclear quantum effects, by using a series of different flavors of thermodynamic integration. As an example, for the two most stable forms of paracetamol we find that anharmonic contributions, different descriptions of van der Waals interactions, and nuclear quantum effects **all** matter to quantitatively determine the stability of different phases [1]. Our studies indicate that anharmonic free energies could play an important role for molecular crystals composed by large molecules and opens the way for a systematic inclusion of these effects in order to obtain a predictive screening of structures.
[1] Rossi, Gasparotto, Ceriotti, *PRL* **117**, 115702 (2016).

TT 52.4 Wed 15:45 GER 38

Exact solutions and approximations in the exact factorization of the electron-nuclear wavefunction — •Graeme Gossel and Neepa Maitra — Department of Physics and Astronomy, Hunter College of the City University of New York, 695 Park Avenue, New York, NY 10065.

"Recently it was shown how a molecular wavefunction may be written exactly as a single product of a nuclear and an electronic wavefunction, with a pair of corresponding equations of motion [1]. This exact factorization provides a new and rigorous starting point for developing intuitive and physical approximations to the exact coupled system. Strikingly, in this factorized picture the electronic Hamiltonian is not strictly Hermitian. Nevertheless, the norm is conserved so long as certain terms persist. This, and other constraints, inform the approximations we apply to make the process numerically feasible. In parallel we present numerical self-consistent solutions of the exact factorization equations devoid of approximations to assess accuracy and behaviour of different terms. Finally, we discuss how a well characterized and robust single-product-picture such as this may be used in TDDFT calculations.
[1] A Abedi, NT Maitra, and EKU Gross, PRL 105 (12), 123002, 2010

TT 52.5 Wed 16:00 GER 38

Insight into time-propagation TDDFT excitations via Kohn–Sham decomposition — •Tuomas P. Rossi[1], Mikael Kuisma[2,3], Martti J. Puska[1], Risto M. Nieminen[1], and Paul Erhart[2] — [1]Aalto University, Espoo, Finland — [2]Chalmers University of Technology, Gothenburg, Sweden — [3]University of Jyväskylä, Jyväskylä, Finland

The real-time-propagation formulation of time-dependent density-functional theory (RT-TDDFT) is an efficient method for calculating optical excitations of large molecules and nanoparticles. However, within RT-TDDFT, the analysis of the response is often limited to photoabsorption spectra and induced densities, in contrast to linear-response formulations of TDDFT, such as the Casida method, in which one can obtain further understanding on the basis of the Kohn–Sham electron-hole decomposition of the excitations.

In this work, we show that the Kohn–Sham decomposition can be equivalently obtained from RT-TDDFT calculations. We demonstrate the approach for the optical response of organic molecules and large metallic nanoparticles. The focus is especially on plasmonic applications, for which the method enables the analysis in terms of transition contribution maps [1]. By using the decomposition, we can shed light on the microscopic origin of plasmon resonances and their damping via plasmon–single-electron coupling, while retaining the favorable scaling of RT-TDDFT compared to linear-response formulations.
[1] S. Malola *et al.*, ACS Nano **7**, 10263 (2013).

TT 52.6 Wed 16:15 GER 38

Gauge-invariant Magnetic Properties from Time-Dependent

Current-Density-Functional Theory — •Nathaniel Raimbault[1], Paul de Boeij[3], Pina Romaniello[2], and Arjan Berger[1] — [1]Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université Toulouse III - Paul Sabatier — [2]Laboratoire de Physique Théorique, CNRS, IRSAMC, Université Toulouse III - Paul Sabatier — [3]University of Twente, Faculty of Science and Technology, Physics of Interfaces and Nanomaterials

Standard formulations of magnetic response properties are often plagued by gauge dependencies, which can lead to unphysical results, and to a slow convergence with basis-set size. In this talk we present a novel method for obtaining magnetic properties from the current density [1]. This alternative scheme is fully gauge-invariant, numerically efficient, and can be applied to any method from which the current density can be obtained. To illustrate our method, we applied it to time-dependent current-density-functional theory (TDCDFT). While different types of magnetic properties can be calculated in this way, we here emphasize the calculation of circular dichroism spectra, which are notably important in order to characterize secondary structures in biomolecules. The circular dichroism spectra we thus obtain for methyloxirane, dimethyloxirane and α-pinene are in good agreement with experiment [2]. [1] N. Raimbault, P.L. de Boeij, P. Romaniello, and J.A. Berger, PRL 114, 066404 (2015); [2] N. Raimbault, P.L. de Boeij, P. Romaniello, and J.A. Berger, JCTC 12, 3278 (2016)

TT 52.7 Wed 16:30 GER 38

Calculation of charge transfer integrals using constrained-DFT — •Tobias Lettmann and Nikos Doltsinis — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Deutschland

For the investigation of charge transport properties of organic semiconductor materials, the fast and accurate calculation of charge transfer integrals (or transition matrix elements) is desirable. It has been suggested that the transfer integrals depend on a universal linear function of the corresponding wavefunction overlap, which can then be used to approximate the integral at a reduced computational cost[1].

We have calculated transfer integrals for dimers of poly(3-hexylthiophene) (P3HT) and diperylene bisimide (DiPBI), which are used in organic solar cells, in a large variety of intra- and intermolecular conformations and polymer lengths using a constrained-DFT approach[2]. Our results show, that there is indeed a universal relation between transfer integral and wavefunction overlap. However this relation is (i) nonlinear for large overlaps and (ii) only holds true if the transfer integral is rescaled by the number of electrons of the respective system.

[1] F. Gajdos et al.: *J. Chem. Theory Comput.*, 2014, **10**, 4653
[2] H. Oberhofer, J. Blumberger: *J. Chem. Phys.*, 2010, **133**, 244105

TT 52.8 Wed 16:45 GER 38

Towards ultra long-range ab-initio calculations — •Tristan Müller[1], Sangeeta Sharma[1,2], Eberhard K.U. Gross[1], and John K. Dewhurst[1] — [1]Max-Planck-Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — [2]Department of physics, Indian Institute for Technology-Roorkee, 247997 Uttarkhand, India

We propose a generalization of the Bloch state which involves an additional sum over a finer grid in reciprocal space around each k-point. This allows for ab-initio calculations of ultra long-range modulations in the density which may involve millions of unit cells but with an efficiency rivaling that of a single unit cell. This is due to a new algorithm developed specifically for solving the particular eigenvalue problem that this ansatz requires. Thus physical effects on the micron length scale, which nevertheless depend on details of the electronic structure on nanometer length scales, can be computed exactly within density functional theory.

TT 52.9 Wed 17:00 GER 38

Local density fitting within a Gaussian and plane waves scheme for large-scale density functional theory calculations — •Dorothea Golze[1,2], Marcella Iannuzzi[1], and Jürg Hutter[1] — [1]Aalto University, Otakaari 1, 02150 Espoo, Finland — [2]University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland

A local resolution-of-identity (LRI) approach is introduced in the Gaussian and plane waves (GPW) scheme to enable large-scale Kohn-Sham (KS) density functional theory calculations. The construction of the KS matrix in GPW scales already linearly with respect to system size by using a plane wave expansion of the density for the evaluation of the Coulomb term in combination with a local basis. The intention is to retain the linear scaling of the GPW approach, while reducing the prefactor for computing the KS matrix. The locality of the density fitting ensures an $O(N)$ scaling and is implemented by approximating the atomic pair density by an expansion in one-center fit functions. The prefactor is smaller with LRI since the computational demands for the grid-based operations become negligible, while they are dominant in GPW. We observe a speed-up of the self-consistent field (SCF) procedure by a factor of up to 30 for periodic systems dependent on the symmetry of the simulation cell and the grid cutoff. The accuracy of LRIGPW is assessed for different systems and properties. Generally, total energies, reaction energies, intramolecular and intermolecular structure parameters are well reproduced. LRIGPW yields also high quality results for extended condensed phase systems such as liquid water, ice XV and molecular crystals.

TT 52.10 Wed 17:15 GER 38

From the Electron Localization Function to a Coalescent-Pair Locator — •Stefano Pittalis[1], Daniele Varsano[1], Alain Delgado[2,3], and Carlo Andrea Rozzi[1] — [1]Istituto Nanoscienze, Consiglio Nazionale dellle Ricerche, Via Campi 213a, 41125 Modena, Italy — [2]Department of Physics, University of Ottawa, Ottawa, ON K1N 6N5, Canada — [3]Centro de Aplicaciones Tecnológicas y Desarrollo Nuclear, Calle 30 # 502, 11300 La Habana, Cuba

The Electron Localization Function (ELF), as proposed originally by Becke and Edgecombe, uses the information on the distribution of pairs of electrons with parallel spins. The ELF has been widely adopted as a descriptor of atomic shells and covalent bonds, but it is not useful to visualize the bond in H_2 – the simplest neutral molecule in the universe. Here we propose a complementary descriptor which also works for H_2 by exploiting the information on pairs of electrons with opposite spins. Remarkably, only quantities derived from occupied single-particle orbitals are required in the calculations. If time allows, implications for developing improved approximate density functionals will also be discussed.

TT 52.11 Wed 17:30 GER 38

Band structure interpolation via maximally localized Wannier functions implemented in LAPW+lo basis — •Sebastian Tillack, Andris Gulans, and Claudia Draxl — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin

The band structure is one of the most fundamental quantities of any solid that carries a lot of information about the material's properties. Obtaining a smooth dispersion from density-functional theory (DFT) and especially from the *GW* approximation of many-body perturbation theory may be very expensive. To this extent, we have implemented a method for generating maximally localized Wannier functions (WF) [1] from Kohn-Sham wavefunctions in the full-potential all-electron code `exciting` [2] using a (linearized) augmented plane-waves plus local-orbitals basis. These WF are used for interpolating wavefunctions and corresponding eigenenergies for arbitrary **k**-points in a computationally cheap post-processing step. The interpolated Kohn-Sham and *GW* bands of conventional and two-dimensional semiconductors and insulators are also used as an input to calculations of optical-excitation spectra.

[1] N. Marzari and D. Vanderbilt, *Phys. Rev. B* ***56***, 12847 (1997)
[2] A. Gulans, et al. *J. Phys.: Condens. Matter* ***26***, 363202 (2014)

TT 52.12 Wed 17:45 GER 38

Chemical insight from Fermi-Löwdin orbitals — •Torsten Hahn[1], Sebastian Schwalbe[1], Simon Liebing[1], Jens Kortus[1], and Mark Pederson[2] — [1]Institute for Theoretical Physics, TU Freiberg, Germany — [2]Department of Chemistry, Johns Hopkins University, Baltimore Maryland (MD), US

The recently developed Fermi-Löwdin orbital based method for correcting the self-interaction error in Density Functional Theory (FLO-SIC DFT) [1,2,3] is briefly introduced. Contrary to standard DFT approaches, where only auxiliary Kohn-Sham orbitals are available, FLO-SIC DFT delivers a set of well-defined, localised Fermi-Löwdin orbitals. These localised orbitals together with their optimised reference positions yield an inherently 'chemical' representation of bonding details in molecules that resembles remarkably well Lewis concept of lone and binding electron pairs. For complex examples, the method provides detailed insights into the bonding situation in terms of multi-center many-electron bonds in a natural, chemically-intuitive fashion.

[1] M. R. Pederson et al., JCP 140, 121103 (2014).
[2] M. R. Pederson, JCP 142, 064112 (2015).
[3] T. Hahn et al., JCP 143, 224104 (2015).

TT 52.13 Wed 18:00 GER 38

Conditions for describing triplet states in reduced density matrix functional theory — Iris Theophilou[1], Nektarios N. Lathiotakis[2], and •Nicole Helbig[3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vass. Constantinou 48, GR-11635 Athens, Greece — [3]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

We consider necessary conditions for the one body-reduced density matrix (1RDM) to correspond to a triplet wave-function of a two electron system. The conditions concern the occupation numbers and are different for the high spin projections, $S_z = \pm 1$, and the $S_z = 0$ projection. Hence, they can be used to test if an approximate 1RDM functional yields the same energies for both projections. We employ these conditions in reduced density matrix functional theory calculations for the triplet excitations of two electron systems. In addition, we propose that these conditions can be used in the calculation of triplet states of systems with more than two electrons by restricting the active space. We assess this procedure in calculations for a few atomic and molecular systems. We show that the quality of the optimal 1RDMs improves by applying the conditions in all the cases we studied.

TT 53: Poster Session: Superconductivity 1

Time: Wednesday 15:00–19:00 Location: P2-OG2

TT 53.1 Wed 15:00 P2-OG2

Disorder-driven insulating transition in few-layer $NbSe_2$ crystals. — •Nicola Paradiso, Andreas Eller, Tobias Scharff, Sofia Blanter, and Christoph Strunk — Institut für Experimentelle und Angewandte Physik, University of Regensburg

We investigate the impact of disorder on the transport characteristics of few-layer thick crystals of $NbSe_2$. This type II superconducting material is an interesting playground for the study of superconductivity in two dimensions. Recent experiments have demonstrated that in the low-disorder regime superconductivity can be observed even in the single-layer limit. Our measurements go in the opposite direction: we show that in the regime of high disorder a sharp resistance upturn is observed at low temperature. The insulating transition temperature is close to the critical temperature for the superconducting transition of clean $NbSe_2$ crystals. Our results indicate that single crystals behave in a similar way as metal films.

TT 53.2 Wed 15:00 P2-OG2

Superconducting properties of $[(SnSe)_{1+\delta}]_m[NbSe_2]_1$ ferecrystals — •Martina Trahms[1], Corinna Grosse[1], Olivio Chiatti[1], Kyle Hite[2], Matti B. Alemayehu[2], Dave J. Johnson[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Department of Chemistry and Material Science Institute, University of Oregon, Eugene, Oregon 97403, United States

Recently much attention has been paid to the electrical properties of monolayers of the superconducting transition metal dichalcogenide $NbSe_2$ and especially on the influence of the dimensional cross-over. Because thin films are very sensitive to external influences, buried superconducting layers such as ferecrystals are of great interest. Ferecrystals are turbostratically disordered layered systems in which the involved materials are alternately stacked in a repeated sequence. This experimental work investigates the Ginzburg-Landau coherence length of $[(SnSe)_{1+\delta}]_m[NbSe_2]_1$ ferecrystals. In particular, whether two dimensional superconductivity can be established in these systems. By changing the SnSe content between 1 and 6 bilayers of SnSe, the distance of the superconducting $NbSe_2$ monolayers was increased, resulting in repeat unit distances between 1.25 nm and 4.14 nm. The coupling of the $NbSe_2$ layers was investigated by determining the out-of-plane Ginzburg-Landau coherence lengths by electrical transport measurements in a magnetic field closely below the transition temperature. A dimensional cross-over could not be identified; however, a decoupling trend with increasing distance of the $NbSe_2$ layers was observed.

TT 53.3 Wed 15:00 P2-OG2

Rhenium-molybdenum coplanar superconducting electronics compatible with carbon nanotube growth — •Stefan Blien, Karl J. G. Götz, Thomas Huber, Niklas Hüttner, Wolfgang Himmler, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

At low temperature, carbon nanotubes act as quantum dots as well as nano-electromechanical resonators. By growing them in a last fabrication step over pre-existing chip structures, one obtains "ultraclean" devices, displaying high mechanical quality factors as well as unperturbed electronic transport spectra. For integrating such structures with superconducting coplanar circuits, superconductors that withstand the nanotube CVD growth process are needed.

We compare rhenium-molybdenum alloys of different composition and different deposition technique, regarding their material composition and both dc and GHz electronic properties. The rhenium-molybdenum thin films still display superconductivity after the CVD process, with critical temperatures up to $T_c \simeq 8\,\mathrm{K}$. Coplanar waveguide resonators with $Q_i \simeq 5000$ at dilution refrigerator temperature are characterized and and dissipation mechanisms discussed.

TT 53.4 Wed 15:00 P2-OG2

Incommensurate magnetism of hole-doped cuprates in the normal phase: a LDA+(C)DMFT study — •Amin Kiani and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

In order to investigate the magnetic incommensurate structures in hole-doped cuprates, we calculate the static lattice magnetic susceptibility $\chi(\mathbf{q};0)$ of the single-band t-t' Hubbard model in the normal phase. The calculations are performed via the local density approximation+(cluster) dynamical mean-field theory (LDA+(C)DMFT), following the implementation presented in Ref. [1]. Within this approach we study the effect of the next-nearest-neighbor hopping t' and the Coulomb interaction U as a function of the filling. We will show our results for the representative case $La_{2-x}Sr_xCuO_4$ (LSCO), and compare with available experiments.

[1] A. Kiani and E. Pavarini, Phys. Rev. B **94**, 075112 (2016)

TT 53.5 Wed 15:00 P2-OG2

Properties of self-consistent random matrices: A Case study for the superconductor-insulator transition — •Matthias Stosiek and Ferdinand Evers — University of Regensburg, Germany

Our general interest is in the properties of ensembles of random Hamiltonians that satisfy a self-consistency property. Such ensembles typically appear in mean-field treatments of interacting systems. The example we here consider is the Superconductor Insulator Transition (SIT) where the superconducting gap is calculated self-consistently in the presence of short-range disorder. Our focus is on disordered films with conventional s-wave pairing that we study numerically employing the negative-U Hubbard model within the standard BogoliubovdeGennes approximation. The general question that we would like to address here concerns the auto-correlation function of the pairing amplitude: How does it decay in real space and in what way does it change across the SIT? This poster presents our first (preliminary) results. We speculate that our research might have significant impact on the understanding of the SIT if it turns out that the pairing amplitude decays in a power-law fashion (with exponent below two) at the critical point.

TT 53.6 Wed 15:00 P2-OG2

Unconventional superconductivity in the organic charge transfer salts beyond the Random Phase Approximation — •Karim Zantout and Roser Valentí — Institut für Theoretische Physik, Goethe-Universität Frankfurt am Main, Max-von-Laue-Straße

1, 60438 Frankfurt am Main, Germany

The κ-type organic charge transfer salts are often described by a single-band Hubbard model of dimers on an anisotropic triangular lattice at half filling. This work combines *ab initio* density functional theory calculations and the Two-Particle-Self-Consistent approach to calculate the superconducting transition temperature T_c and the symmetry of the superconducting gap function for some material representatives. Our results show that the dimer model is not sufficient to describe transition temperatures and gap symmetries in these systems and one has to invoke molecular-based models.

TT 53.7 Wed 15:00 P2-OG2

Ferroelectric quantum phase transition inside the superconducting dome of Ca doped $SrTiO_{3-x}$ — •Lin Xiao — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln — LPEM, ESPCI, 10 Rue Vauquelin, 75005 Paris, France

Ferroelectricity and superconductivity are mutually exclusive. Ferroelectricity implies the alignment of electric dipoles in an insulator, and while superconductivity requires pairing of mobile electrons in a metal. However, recently a number of 'ferroelectric metals' have emerged during the past few years (See for example Nature Materials 12, 1024 (2013)). By employing a variety of experimental probes (electric conductivity, electric permittivity, Raman spectroscopy, thermal expansion and sound velocity), we find that calcium doped oxygen-reduced $SrTiO_3$, is the first solid in which ferroelectric-like and superconducting phase transitions occur one after each order.

A variety of superconducting domes have been found in the vicinity of a competing order during the past three decades. In this context, we find evidence for interplay between superconductivity in strontium titanate and a neighboring ferroelectric order. When the ferroelectric order is destroyed by doping, the superconducting critical temperature enhances. This observation may be the first experimental signature of a role played by ferroelectric quantum criticality in the formation of Cooper pairs.

TT 53.8 Wed 15:00 P2-OG2

Superconducting penetration depth measurement and zero field muon spin relaxation experiments under uniaxial strain in Sr_2RuO_4 — •Shreenanda Ghosh[1], Rajib Sarkar[1], Hubertus Luetkens[2], Clifford Hicks[3], and Hans-Henning Klauss[1] — [1]Institute for Solid State Physics, TU Dresden, Dresden, Germany — [2]Paul Scherrer Institute, Villigen, Switzerland — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

We present zero-field muon spin relaxation (μSR) data on the unconventional superconductor Sr_2RuO_4 under uniaxial pressure. Results from previous μSR studies on unstressed Sr_2RuO_4 indicate a spontaneous magnetisation in the superconducting state [1], that has been associated with a time reversal symmetry breaking order parameter, $p_x \pm ip_y$.

The superconducting T_c of Sr_2RuO_4 has been shown experimentally to be sensitive to uniaxial pressure [2], so for more information about the complex superconducting order parameter, we investigate pressurized Sr_2RuO_4 by μSR. For this purpose, we have developed a dedicated device, which offers in situ uniaxial strain tuning via piezoelectric stacks.

[1] G. M. Luke et al., Nature **394**, 558 (1998)
[2] C. W. Hicks et al., Science **344**, 283 (2014)

TT 53.9 Wed 15:00 P2-OG2

Ferromagnetic order and superconductivity in new 1144 iron-based superconductors investigated with NMR — •Felix Brückner[1], Rajib Sarkar[1], Yi Liu[2], Guang-Han Cao[2], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, Technische Universität Dresden, Dresden, Germany — [2]Department of Physics, Zhejiang University of Science and Technology, Hangzhou, China

The recent discovery of two new iron-based superconductors – the so-called 1144 systems – enriches the list of ferromagnetic superconductors. These compounds crystallize in a structure similar to 122 systems. The unique feature is that adjacent interlayers contain different atoms. In our case two systems (Rb/Cs)$EuFe_4As_4$ are investigated with NMR to clarify the interplay between superconductivity and Eu-ferromagnetism. We present caracterization data as well as NMR spectroscopy and relaxation data.

TT 53.10 Wed 15:00 P2-OG2

Crystal growth and characterization of NdFeAs(O,F) — •Agnes Adamski, Mahmoud Abdel-Hafiez, and Cornelius Krellner — Physikalisches Institut, Goethe University Frankfurt

Since the discovery of iron-based superconductors, much effort was put on the crystal growth of the various systems and their characterization. Although, the initial flurry of activities was mainly performed on the so-called 1111 systems, the focus has been rapidly shifted towards other materials, were large high-quality single crystals are available. In contrast, the growth of sizable high-quality single crystals of 1111 compounds is extremely challenging, slowing down the scientific progress in this type of compounds.
Here, we report on the crystal growth of fluorine doped NdFeAsO under ambient pressure conditions by using the flux-growth technique. With this method we were able to grow single crystals up to 800 μm size and with superconducting transitions temperatures above 50 K. Subsequently, the obtained samples were analyzed with powder diffractometry, electron probe micro analysis, magnetic and transport measurements to determine the structural and physical properties. Using high-pressure electric resistance measurements on these crystals, we demonstrate a tentative $p-T$ phase diagram.

TT 53.11 Wed 15:00 P2-OG2

Detecting sign-changing superconducting gap in LiFeAs using quasiparticle interference — •Dustin Altenfeld[1], Peter J. Hirschfeld[2], Igor I. Mazin[3], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Department of Physics, University of Florida, Gainesville, Florida 32611, USA — [3]Code 6393, Naval Research Laboratory, Washington, DC 20375, USA

We present quasiparticle interference (QPI) measurement in Fe-based superconductors as a robust way of determining the superconducting gap sign structure in experiment. We show that the bias dependence of the signed symmetrized and antisymmetrized QPI maps are useful to obtain a characteristic signature of a gap sign change or lack thereof, starting from two-band model up to ab initio based band structure calculation. The experimental realization of the suggested method was successfully realized in FeSe, where a sign changing gap sign structure was identified. We provide a motivation for the application to the LiFeAs compounds.

TT 53.12 Wed 15:00 P2-OG2

Spin resonance of $Ba_{1-x}K_xFe_2As_2$ studied by neutron scattering — •Chul-Ho Lee[1], Kunihiro Kihou[1], Jitae Park[2], Kazumasa Horigane[3], Florian Wasser[4], Navid Qureshi[5], Yvan Sidis[6], Jun Akimitsu[3], and Markus Braden[4] — [1]AIST, Japan — [2]MLZ, Germany — [3]Okayama Univ., Japan — [4]Universitat zu Koln, Germany — [5]ILL, France — [6]LLB, France

The remarkable enhancement of magnetic neutron scattering signals appearing in a superconducting phase, so called spin resonance, is important to examin since it could include information of Cooper pairing. Here, we examined the spin fluctuation of hole-doped $Ba_{1-x}K_xFe_2As_2$ by inelastic neutron scattering to clarify the doping dependence of spin resonance. Neutron scattering experiments were conducted using the triple-axis spectrometer PUMA at FRM ll, Germany and 2T1 at LLB, France. We have found that the behavior of the spin resonance dramatically changes around x = 0.66 [1]. Resonance peaks have been observed clearly below 2Δs in the optimum doping region, while they are absent in the overdoped region. Instead, there is a transfer of spectral weight from energies below 2Δs to higher energies, peaking at values of 3Δs for x = 0.84. These results indicate a reduced impact of magnetism on Cooper pair formation in the overdoped region.

[1] C. H. Lee et al., Sci. Rep. 6, 23424 (2016)

TT 53.13 Wed 15:00 P2-OG2

Fermi-surface topology of $(Rb,Cs)Fe_2As_2$ — •Tobias Förster[1], Johannes Klotz[1], Kathrin Götze[1], Seunghyun Khim[2], Helge Rosner[2], and Jochen Wosnitza[1] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The unique Fermi-surface topology of many iron-pnictide superconductors stimulates a number of theories on the nature of the pairing interactions in these materials. In the case of $(K,Rb,Cs)Fe_2As_2$, there is an ongoing discussion whether a Lifshitz transition is connected to the superconducting properties of these 122 iron arsenides. Studies of the pressure dependence of H_{C2} did not find evidence for that kind

of transition [1,2]. In contrast, high-resolution band structure calculations show a van-Hove singularity close to the Fermi energy, favouring a Lifshitz transition. In order to investigate the possible impact of this feature, a precise knowledge of the electronic structure is eminent. We, therefore, calculated the Fermi surface of (Rb,Cs)Fe_2As_2 using the full-potential-local-orbital scheme and started investigating the de Haas-van Alphen effect of (Rb,Cs)Fe_2As_2 in static fields up to 18 T. In our contribution, we show the first results of our ongoing torque-magnetometry measurements and compare them with the results of our band-structure calculations.

[1] F. F. Tafti *et al.*, Phys. Rev. B. **89** 134502 (2014).
[2] F. F. Tafti *et al.*, Phys. Rev. B. **91** 054511 (2015).

TT 53.14 Wed 15:00 P2-OG2

Magnetic properties and electronic correlations in $BaTM_2As_2$ (TM=Cr, Mn, Fe, Co, Ni, Cu, Zn) — •Francesco Scaravaggi[1], Sebastian Selter[1], Rhea Kappenberger[1], Saicharan Aswartham[1], Sabine Wurmehl[1], Anja U.B. Wolter[1], and Bernd Büchner[1,2] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069, Dresden, Germany

In order to better understand the multi-orbital nature of Fe-based superconductors in combination with strong electronic correlations in this class of materials, we report on a systematic investigation of the magnetic and thermodynamic properties of the isostructural series $BaTM_2As_2$ (TM=Cr, Mn, Fe, Co, Ni, Cu, Zn). Magnetization, specific heat and dilatometry measurements were performed on single crystalline samples to investigate the changes in the electronic and magnetic character and the degree of electronic correlation, varying the average occupancy of the 3d shell as a control parameter within the series. The results show that upon changing the occupation of the 3d orbitals, the electronic and magnetic character changes dramatically, which suggests a very complex interaction between on-site Coulomb repulsion, Hund's coupling and other competing effects.

This work has been supported by Graduiertenkolleg GRK 1621.

TT 53.15 Wed 15:00 P2-OG2

High field properties of superconducting $Ba(Fe_{1-x}Ni_x)_2As_2$ thin films — •Stefan Richter[1,2], Fritz Kurth[1], Kazumasa Iida[3], Kirill Pervakov[4], Aurimas Pukenas[2], Saicharan Aswartham[1], Chiara Tarantini[5], Jan Jaroszynski[5], Jens Hänisch[6], Vadim Grinenko[1,2], Sabine Wurmehl[1], Werner Skrotzki[2], Bernd Büchner[1,2], Kornelius Nielsch[1,2], and Ruben Hühne[1] — [1]IFW, Dresden — [2]TU Dresden — [3]Nagoya University, Japan — [4]RAS, Moscow, Russia — [5]NHMFL, Tallahassee, USA — [6]KIT, Karlsruhe

The Fe based superconductors show great potential for high field applications due to their high upper critical field, their small anisotropy and their increased tolerance to small angle grain boundaries. The study of Fe-based superconducting thin films contributes to a better understanding of these correlated electron systems. We present results for epitaxial $Ba(Fe_{1-x}Ni_x)_2As_2$ thin films, which have been grown with pulsed laser deposition. The behavior of the upper critical field and critical current density has been measured in high magnetic fields up to 35 T. We find an increased slope of the upper critical field near T_c and compared to Co-doped thin films a smaller vortex liquid phase at low temperatures.

TT 53.16 Wed 15:00 P2-OG2

Doping effect of Mn impurities on the physical properties of optimally electron doped $Sr(Fe_{0.86}Co_{0.14})_2As_2$ — •Luminita Harnagea, Giri Mani, and Surjeet Singh — Indian Institute of Science Education and Research, Pune - 411008, India.

Using transport and magnetization measurements we studied the effect of Mn doping in optimally electron doped $Sr(Fe_{0.86}Co_{0.14})_2As_2$ single crystal. The as - grown $Sr(Fe_{0.86}Co_{0.14})_2As_2$ single crystal exhibits a superconducting transition temperature (T_c) of around 15 K. Doping with Mn at the Fe site in $Sr(Fe_{0.86}Co_{0.14})_2As_2$ leads to a gradual suppression of the transition temperature with an initial rate of about ΔT_c 5 K per Mn percentage. The residual resistivity of the doped samples increases with increasing Mn concentration. The low-temperature magnetic susceptibility of the Mn-doped samples exhibits a Curie tail, which gets progressively enhanced with increasing Mn - concentration, suggesting that the Mn - ions carry a localized magnetic moment consistent with S = 1/2 local moment. The paramagnetic Mn moments act as Cooper pair-breakers resulting in a gradual suppression of T_c, analogous to $Ba(Fe_{1-x-y}Co_xMn_y)_2As_2$ series of compounds [1]. These results are, however, in stark contrast with the case of Mn doped $LaFeAsO_{0.89}F_{0.11}$, where a Mn concentration as small as 0.2 %, suppresses the superconductivity completely [2]. These differences are rather surprising and their more detailed understanding might throw light on the nature of superconducting state in iron pnictides.

[1] D. LeBoeuf et al., Phys. Rev. B 89, 035114 (2014)
[2] F. Hammerath et al., Phys. Rev. B 89, 134503 (2014)

TT 53.17 Wed 15:00 P2-OG2

Magnetic and electric characterization of bulk FeSe superconductors with Ag addition — Thomas Karwoth[1], •XianLin Zeng[1], Koichi Furutani[1,2], Alex Wiederhold[1], Michael Koblischka[1], M Muralidhar[2], M Murakami[2], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, Saarland University, Campus C 6 3, 66123 Saarbrücken, Germany. — [2]Superconducting Materials Laboratory, Department of Materials Science and Engineering, Shibaura Institute of Technology, 3-7-5 Toyosu, Koto-ku, Tokyo 135-8548, Japan

Superconductivity of bulk FeSe samples was characterized through magnetic and electric measurements. In order to improve the superconducting properties, the sintering temperature was varied up to 900 oC and to improve the connectivity, silver was applied in low concentrations to the samples ranging from 0 to 7%. The electric properties of the samples were investigated by the four point probe method (R-T measurement and V-I characteristics). Generally, the sample with 4The magnetic properties (M-T and M-H) of the samples were measured using an extraction magnetometer in a Quantum Design PPMS with fields up to 7 T. The critical current densities and the flux pinning forces were estimated using the extended Bean model, extending the work published in [1].

[1] M. Muralidhar et al., Phys. stat. solidi (a), DOI 10.1002/pssa.201600299.

TT 53.18 Wed 15:00 P2-OG2

High field ^{77}Se NMR on single crystalline FeSe. — •Sebastian Molatta[1,2,3], Z. T. Zhang[1,4], R. Sarkar[2,3], P. Biswas[5], T. Wolf[6], H. v. Löhneysen[6], J. Wosnitza[1,2,3], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]IFP, Technical University of Dresden, Germany — [3]DFG GRK 1621 — [4]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [5]Paul-Scherrer-Institute, Switzerland — [6]IFP, Karlsruhe Institute of Technology, Germany

FeSe is currently discussed as a superconductor in the crossover regime between the weakly coupled Bardeen-Cooper-Schrieffer (BCS) and the strongly coupled Bose-Einstein-condensate (BEC) limit. In particular, at high magnetic fields, the energies of the Zeeman interaction, superconducting gap, and the Fermi temperature are comparable in FeSe. We report recent results of the spin susceptibility and low-energy quasiparticle excitations probed by means of nuclear magnetic resonance (NMR) spectroscopy in the highly spin-polarized state close to the upper critical field of superconductivity. The superconducting state is evidenced by a reduced radio-frequency penetration depth reflected by a decreasing NMR signal intensity towards low temperatures. The spin-lattice relaxation rate points towards a field-induced change of the gap structure within the superconducting state.

TT 53.19 Wed 15:00 P2-OG2

Disorder-promoted C_4-symmetric magnetic order in iron-based superconductors — •Mareike Hoyer[1], Rafael M. Fernandes[2], Alex Levchenko[3], and Jörg Schmalian[1] — [1]Institut für Theorie der Kondensierten Materie und Institut für Festkörperphysik, Karlsruher Institut für Technologie, Deutschland — [2]School of Physics and Astronomy, University of Minnesota, USA — [3]Department of Physics, University of Wisconsin-Madison, USA

In most iron-based superconductors, the transition to the magnetically ordered state is closely linked to a lowering of structural symmetry from tetragonal (C_4) to orthorhombic (C_2). However, recently, a regime of C_4-symmetric magnetic order has been reported in certain hole-doped compounds. This novel magnetic ground state can be understood as a double-**Q** spin density wave, and depending on the relative orientations of the two order parameters $\mathbf{M}_1$ and $\mathbf{M}_2$, either a noncollinear spin-vortex crystal (SVC) or a nonuniform charge-spin density wave (CSDW) could form. Experimentally, CSDW has been established as the magnetic configuration of some of these optimally hole-doped compounds, whereas in low-energy itinerant models SVC and CSDW

states are nearly degenerate. Extensions of these low-energy models including additional electronic interactions even tip the balance in favor of the SVC, in apparent contradiction with the recent experimental findings.

Here, we revisit the phase diagram of magnetic ground states of low-energy multi-band models in the presence of weak disorder. We show that impurity scattering not only promotes the transition from C_2 to C_4-magnetic order, but also favors the CSDW over the SVC phase.

TT 53.20 Wed 15:00 P2-OG2

Tetragonal magnetic order and superconductivity in iron pnictides — •Chris Koschenz and Carsten Timm — Institute of Theoretical Physics, Technische Universität Dresden

Multiband and multiorbital physics is crucial for understanding superconductivity and magnetism in iron pnictides. We employ a realistic multiorbital model to study the newly discovered tetragonal magnetic phase in $Ba_{x-1}Na_xFe_2As_2$ and $Ba_{1-x}K_xFe_2As_2$.This additional four-fold symmetric phase is observed in $Ba_{x-1}Na_xFe_2As_2$ by neutron powder diffraction close to the suppression of the spin-density-wave (SDW) order and is in agreement with the scenario of magnetically driven nematic order.

We elucidate the role played by orbital effects and compare them to other multiorbital systems. Furthermore, we study the coexistence and competition of tetragonal magnetic order and superconductivity as well as the possibility of additional phase transitions in this regime.

TT 53.21 Wed 15:00 P2-OG2

Constraints on the total coupling strength to bosons in the Fe based superconductors — •Stefan-Ludwig Drechsler[1], Helge Rosner[2], Vadim Grinenko[3], and Steve Johnston[1,4] — [1]Leibniz-Institute IFW-Dresden, D-01171 dresden, Germany — [2]Max-Planck Institute f. Chemical Physics of Solids, Dresden, Germany — [3]TU Dresden, Dresden, Germany — [4]Deptm. of Physics and Astronomy, University of Tennesee, Knoxville 37996, USA

There is still no consistent interpretation of the normal state of Fe based superconductors (FeSC) properties, where the strength of the el-el interaction and the role of correlation effects are under debate. Based on empirical observations and qualitative insight from DFT calculations, we show that the superconducting and low-energy thermodynamic properties of the FeSC can be described semi-quantitively within multiband Eliashberg-theory. An important high-energy mass renormalization (MR) is accounted for phenomenologically in accord with constraints provided by thermodynamic, optical, and angle-resolved photoemission data. When viewed in this way, all FeSC with $T_c <$ 40 K studied so far are found to belong to an *intermediate* coupling regime. This is in contrast to strong coupling scenarios proposed in the early period of the FeSC history. We also discuss several related issues, including the role of band shifts as measured by the positions of van Hove singularities, and a recently suggested a quantum critical point in the strongly hole-doped systems AFe_2As_2 (A = K, Rb, Cs). Using high-precision full relativistic GGA-band structure calculations, we arrive at a somewhat milder MR in comparison with other studies.

TT 53.22 Wed 15:00 P2-OG2

Kinetics of quasiparticles in conventional superconductors beyond mean field — •Frank Lengers, Peter Kettmann, Simon Hannibal, and Tilmann Kuhn — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Nonequilibrium dynamics of superconductors offer a versatile tool for understanding the underlying many particle interactions. Conventional superconductors can be excited into the nonadiabatic regime by THz pulses to study the Higgs mode in those materials. Theoretical modelling of those processes is typically done on the mean field level. Here we present a quantum kinetic treatment of the well-known BCS-model for conventional superconductors beyond the mean field approximation. We treat the quasiparticle correlations as independent variables in a density-matrix formalism by truncating the quantum mechanical BBGKY hierarchy at certain order. It is shown that the well-known mean field equations of motion are recovered at the lowest truncation level. The dynamics of a conventional superconductor after excitation into the nonadiabatic regime is modelled by a sudden quench of the coupling parameter of the BCS-model. Thereby we study the Higgs mode in a conventional superconductor and compare the results to the mean field case. In a second part we introduce semiclassical equations of motion. We observe that the resulting changes due to the extension of the model compared to the mean field case are rather small. Yet relaxation and dephasing behaviour of quasiparticles and coherences can be observed.

TT 54: Poster Session: Cryotechnique

Time: Wednesday 15:00–19:00 Location: P2-OG3

TT 54.1 Wed 15:00 P2-OG3

Torque-detected electron spin resonance and torque magnetometry — •Alexey Alfonsov[1], Julian Zeisner[1], Vladislav Kataev[1], and Bernd Büchner[1,2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, IFW Dresden, D-01171 Dresden, Germany — [2]Technische Universität Dresden, D-01062 Dresden, Germany

Magnetic anisotropy is a key property of many materials, which has been under a great interest of scientists from around the world. The magnetic anisotropy is defined by the complex interplay of different degrees of freedom, such as spin or/and orbital moments, charge and lattice. One of the most appropriate methods to study magnetic anisotropies, and related properties is high field and multifrequency electron spin resonance (HF-ESR). Unfortunately samples of many new materials interesting for the investigation are available in very small sizes: in some cases it is complicated to synthesize large crystals, in other cases, the size is a key property of the material itself. This all rises a problem of the detection of the ESR signal from such a small sample, especially in the case of a multifrequency ESR spectrometer, where in order to increase the sensitivity one has to apply restrictions on the microwave frequency, strength and orientation of magnetic field. To overcome this problem we develope a multifrequency cantilever-based (torque-detected) ESR spectrometer, which, additionally, in the absence of the microwave radiation is transformed into a torque magnetometer.

TT 54.2 Wed 15:00 P2-OG3

Design of a 30 mK scanning tunneling microscope for spin-polarized measurements — •Sebastian Schimmel, Danny Baumann, Alexander Horst, Ralf Voigtländer, Dirk Lindackers, Bernd Büchner, and Christian Hess — IFW Dresden, Helmholtzstrasse 20, 01069, Dresden, Germany

We present the concept of a milli-Kelvin scanning tunneling microscope system, which is particularly designed for long term STM/STS and spinpolarized measurements at a base temperature of 30 mK within magnetic fields. The low temperature is provided by a 3He/4He Dilution Refrigerator that allows measurements with very high resolution in energy and real-space for up to 7 days without refilling the liquid helium reservoir. The position of our sample inside the STM is exactly at the center of a 9-4 T vector magnet that gives us the opportunity to systematically study local magnetic structures on the nanoscale by spinpolarized-STM/STS. Furthermore, the setup contains a two-chamber ultra-high-vacuum system for sample/tip preparation and storage. To avoid that any vibrations can be transferred to the STM the whole construction will be held by a two-stage passive/active damping system. With this contribution we would like to show our progress in setting up the mentioned 30 mK STM system.

TT 54.3 Wed 15:00 P2-OG3

A novel bridge-type radio frequency resonator for studying two level system dynamics under electric dc bias at low temperatures — •Sven Lutter, Benedikt Frey, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, D-69120 Heidelberg

The low temperature behavior of solids is well described by the standard tunneling model. Hereby, two level systems (TLS) are the dominant excitation in the solid. TLSs carrying an electric dipole moment couple to external electric fields and consequently can be studied in dielectric experiments. In particular, the application of an electric

dc field is used to provide new insight into the TLS non-equilibrium dynamics.

We have developed a novel bridge-type radio frequency resonator. The capacitors of this resonator are arranged in a Wheatstone bridge-like configuration. Across one bridge diagonal the coil is attached, across the other the dc bias. The resonator is coupled inductively to the feed line and read out by a network analyzer.

We show first results on the optical glass N-BK7 for temperatures between a few millikelvins and several kelvins.

TT 54.4 Wed 15:00 P2-OG3

Development of a novel calorimetry setup based on metallic paramagnetic temperature sensors — •Andreas Reifenberger, Sebastian Kempf, Andreas Fleischmann, Rüdiger Klingeler, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, D-69120 Heidelberg

For the measurement of the specific heat of superconducting mg-sized metallic glass samples in the temperature range down to 10 mK we have developed a new microfabricated platform. It addresses challenging aspects of such a setup like the thermal contact between sample and platform, the necessary thermometer resolution and an addenda heat capacity excceeding that of the samples of interest (typically nJ/K @ 20 mK). Our novel setup is based on the relaxation method, where the thermal relaxation following a well defined heat pulse is monitored to extract the specific heat. The sample platform ($5 \times 5\,\mathrm{mm}^2$) includes a microstructured paramagnetic Ag:Er temperature sensor, which is read out by a dc-SQUID (Superconducting Quantum Interference Device) via a superconducting pickup loop. In this way, a relative temperature precision of $0.5\,\mu$K can be reached. A gold-coated mounting area ($4.4 \times 3\,\mathrm{mm}^2$) is included to improve the thermal contact between sample and platform. The performance of our setup is presented and discussed.

TT 54.5 Wed 15:00 P2-OG3

Novel microstructured superconducting resonator technique for measurements of dielectric polarization echoes — •Anna Pollithy, Andreas Schaller, Sergey Tsurkan, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, D-69120 Heidelberg

The anomalous properties of amorphous solids at low temperatures are governed by tunneling systems, which are theoretically well described as two-level systems in the phenomenological standard tunneling model. These tunneling systems can couple resonantly to electric fields and can be studied by phase coherent methods such as dielectric two-pulse polarization echo measurements.

We have developed a new setup for performing polarization echo experiments on glasses, which is based on microstructured superconducting planar resonators. The resonance frequency and quality factor of such resonators can be predicted with confidence via simulations. Using this setup we aim to carry out echo experiments at different resonance frequencies and short pulse separation time. In the poster we present the new technique and show first experimental results for N-BK7 glass.

TT 54.6 Wed 15:00 P2-OG3

Development of microstructured superconducting resonators for broadband dielectric measurements of N-BK7 glass between 37 MHz and 1 GHz at low temperatures — •Benedikt Frey, Annina Luck, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

The low temperature behavior of amorphous solids is determined by atomic tunneling systems and can be described by the phenomenological standard tunneling model (STM). Over the years, several experimental results showed significant deviations from this model, which led to a number of modifications of this theoretical description, e.g. an interaction between the tunneling systems.

In order to investigate the dielectric susceptibility of glasses in the MHz to GHz range, microstructured superconducting resonators on glass substrates were designed and fabricated. For the first time, such resonators were used for broadband measurements of the real and imaginary part of the dielectric function of the glass N-BK7 between 37 MHz and 1 GHz. A crossover from a one-phonon to a two-phonon based relaxation was observed in this frequency range, which is in accordance with the STM. In this frequency range, comparing low temperature data to the STM, suggests a modified density of states of tunneling systems in this material.

TT 54.7 Wed 15:00 P2-OG3

4 K Pulse Tube Cryocoolers: Solutions for "Dry" Cooling Applications with High Performance Requirements — •Jack-Andre Schmidt[2], Jens Falter[1], Bernd Schmidt[1,2], 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

Within the family of regenerative cooling systems, Pulse Tube Coolers (PTC) provide long life operation and low vibration due to the absence of moving parts inside the cold head. These advantages make PTC's the preferable choice for "dry" cryostats of low noise applications, where maintenance of the system is difficult. However, as a consequence of the periodic compression and expansion cycles of the process gas (Helium), they exhibit - as all cryocoolers - an intrinsic mechanical and thermal variation. In contrast to Gifford-McMahon coolers, PTCs are also bound to operate in vertical orientation. Due to these requirements in distinct cases, an adaption of the PTC to the individual cryostat design becomes necessary. Here we present the successful integration of a PTC into a unique cryostat for an airborne infrared telescope for radio astronomy [2]. Minimizing the intrinsic effects of the PTC down to the noise level of the measurement by suitable damping units is discussed as well as the high performance of the PTC, even operated under the tilting angle of the telescope.

[1] G. Thummes et al., Cryogenics, Vol. 38,3, (1998), 337-342
[2] C. Risacher et al., IEEE Trans. on THz Sci. and Tech., Vol. 6, Issue 2 (2015)

TT 54.8 Wed 15:00 P2-OG3

Effects of thermal non-equilibrium in precision measurements — •Rene Glaser[1], Giles D. Hammond[2], Stefanie Kroker[3], Frank Schmidl[1], and Ronny Nawrodt[1] — [1]Friedrich-Schiller University Jena, Institute for Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]University of Glasgow, Institute for Gravitational Research, University Avenue, Glasgow G12 8QQ, United Kingdom — [3]Physikalisch-Technische Bundesanstalt, Metrology for Functional Nanosystems, Bundesallee 100, 38116 Braunschweig, Germany

Future gravitational wave detectors will very likely utilize silicon-based optics in order to increase their sensitivity. Crucial parts of these detectors, such as suspension elements, will be operated in a thermal non-equilibrium state. We present systematic investigations of the noise relevant properties under thermal non-equilibrium conditions.

TT 54.9 Wed 15:00 P2-OG3

Optical properties of silicon at low temperatures — •Fabian Ritschel[1], Rene Glaser[1], Stefanie Kroker[2], Johannes Dickmann[2], Carol B. Rojas-Hurtado[2], and Ronny Nawrodt[1] — [1]Friedrich-Schiller University Jena, Institute for Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]Physikalisch-Technische Bundesanstalt, Metrology for Functional Nanosystems, Bundesallee 100, 38116 Braunschweig, Germany

Silicon is widely used in semiconductor industry for several optical applications but is also of great interest in optical applications. Especially in precision metrology applications, such as reference cavities or optical components in future gravitational wave detectors, it is currently of great interest. We summarize current efforts in order to investigate several optical parameters of silicon in a wide temperature range from 4.2 K up to 300 K.

TT 55: Poster Session: Superconductivity 2

Time: Wednesday 15:00–19:00 Location: P2-OG3

TT 55.1 Wed 15:00 P2-OG3

Reduction of dissipation in rolled-up superconductor microstructures — E. A. Posenitskiy[1], R. O. Rezaev[1,2], and •V. M. Fomin[3] — [1]Tomsk Polytechnic University, Tomsk, 634050, Russia — [2]Moscow Engineering Physics Institute, Moscow, 115409, Russia — [3]IFW Dresden, Insitute for Integrative Nanosciences, D-01069 Dresden

Vortex dynamics in rolled-up superconductor microtubes [1] are influenced by the interplay between the scalar potential and the inhomogeneous magnetic field component normal to the surface in the presence of a transport current. A numerical solution of the time-dependent Ginzburg-Landau equation coupled with the Poisson equation for the scalar potential allowed us to analyze the potential induced by moving vortices as a function of the transport current. For rolled-up Nb superconductor tubes with radii from 350 nm to 550 nm, the energy dissipation decreases twice as compared to the unrolled planar structures of same dimensions.

The work was supported by the bilateral BMBF-Russia Grant 01DJ13009 and by the COST Action MP1201 "Nanoscale Superconductivity". E. A. P. was supported by the Science Office of the Institute of Physics and Technology at TPU.

[1] V. M. Fomin, R. O. Rezaev, O. G. Schmidt, Nano Lett. **12**, 1282 (2012)

TT 55.2 Wed 15:00 P2-OG3

Spin-Caloritronic Transport in Superconductor-Ferromagnet Tunnel Structures — •Ali Rezaei, Akashdeep Kamra, Peter Machon, and Wolfgang Belzig — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We investigate the effect of an exchange field and spin-flip scattering on the pair potential and the spin Seebeck coefficient of superconductor (S) - ferromagnet (F) hybrid structures using the Green's function method. Such structures have been predicted to show giant charge Seebeck coefficient [1,2]. In the absence of spin-flip scattering, the pair potential of the S has been studied for different values of the exchange field. We show that the normal to S phase transition with decreasing temperature, changes character from second to first order above a certain value of exchange field. The density of states in energy, and spin Seebeck coefficient as a function of temperature have been computed for several values of spin-flip scattering time. We show that spin-flip scattering limits the enhancement in the spin Seebeck coefficient in realistic settings.

[1] P. Machon, M. Eschrig, and W. Belzig, Phys. Rev. Lett. **110**, 047002 (2013)
[2] A. Ozaeta, P. Virtanen, F. S. Bergeret, and T. T. Heikkilä, Phys. Rev. Lett. **112**, 057001 (2014)

TT 55.3 Wed 15:00 P2-OG3

Structural and Magnetic Properties of a Superconducting Spin-Triplet-MRAM Element — •Daniel Lenk[1], Vladimir I. Zdravkov[1,2], Roman Morari[2], Zakir Seidov[3], Yury Khaydukov[4], Aladin Ullrich[1], Günter Obermeier[1], Claus Müller[1], Anatoli S. Sidorenko[2], Hans-Albrecht Krug von Nidda[1], Siegfried Horn[1], Lenar R. Tagirov[1,5], and Reinhard Tidecks[1] — [1]Institut für Physik, Universität Augsburg, D-86158 Augsburg, Germany — [2]D. Ghitsu Institute of Electronic Engineering and Nanotechnologies ASM, MD2028 Kishinev, Moldova — [3]Institute of Physics, Azerbaijan National Academy of Sciences, AZ-1143 Baku, Azerbaijan — [4]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [5]E.K. Zavoisky Physical-Technical Institute of RAS, 420029 Kazan, Russia

We investigated a $Co/CoO_x/Cu_{41}Ni_{59}/Nb/Cu_{41}Ni_{59}$ nanolayered heterostructure, which shows a superconducting transition temperature depending on the magnetic history of the sample. The observed magnetic random access memory (MRAM) element functionality arises from the triplet spin-valve effect, caused by the long-range odd-in-frequency triplet component of superconductivity, obtained at non-collinear relative orientation of ferromagnetic layers. In the present study, we investigate the structural and magnetic properties applying cross-sectional TEM analysis, SQUID magnetometry, FMR spectroscopy and Polarized Neutron Reflectometry (PNR).

TT 55.4 Wed 15:00 P2-OG3

Investigation of Superconducting Proximity and Magnetic Stray Field Effects in Superconductor/Ferromagnet Heterostructures — •Vladimir I. Zdravkov[1,2], Daniel Lenk[1], Roman Morari[2], Zakir Seidov[3], Yury Khaydukov[4], Aladin Ullrich[1], Günter Obermeier[1], Claus Müller[1], Anatoli S. Sidorenko[2], Hans-Albrecht Krug von Nidda[1], Siegfried Horn[1], Lenar R. Tagirov[1,5], and Reinhard Tidecks[1] — [1]Institut für Physik, Universität Augsburg, D-86159 Augsburg, Germany — [2]D. Ghitsu Institute of Electronic Engineering and Nanotechnologies ASM, MD2028 Kishinev, Moldova — [3]Institute of Physics, Azerbaijan National Academy of Sciences, AZ-1143 Baku, Azerbaijan — [4]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [5]E.K. Zavoisky Physical-Technical Institute of RAS, 420029 Kazan, Russia

We have experimentally studied $Nb/Cu_{41}Ni_{59}/nc - Nb/Co/CoO_x$ superconducting spin-triplet spin-valve structures. Due to the proximity effect between the superconductor and the ferromagnets, these structures show a superconducting transition temperature depending on the magnetic configuration of the ferromagnetic layers. Thus, the transition temperatures depend on the magnetic history of the samples, yielding functionality as spin-valves. We observed characteristic features in the magnetoresistance associated with different types of superconducting spin valve effects. To clarify possible influences of stray field effects from Co, we investigate the magnetoresistance of $Nb/Si/Co/CoO_x$ systems.

TT 55.5 Wed 15:00 P2-OG3

Non-equilibrium transport near the disorder-driven SIT — •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, Russia

We have measured the IV characteristics of square shaped TiN films on the superconducting and the insulating side of the superconductor-insulator transition. The superconducting IV characteristics display strong non-linearities including several jumps. The measured data was consistently reproduced in terms of electron heating models ("hotspot theory"), where the thermal conductivity in the superconducting parts of the film and the heat transfer coefficient per unit area to the substrate were used as free fitting parameters. On the basis of the hotspot theory, the obtained value for surface heat transfer coefficient seems to decrease drastically on approach of the disorder-driven SIT. At the same time, the thermal conductivity in the superconducting parts of the film appears to increase significantly on approach of the SIT. Independent thermal conductivity measurements are required to verify this interpretation. On the insulating side of the field-induced SIT the IV characteristics reveal a similar but dual non-linear behaviour. An analysis of the insulating IV characteristics in terms of selfheating in insulating microbridges is a future task.

TT 55.6 Wed 15:00 P2-OG3

Fast and highly sensitive read out electronics for micro-SQUIDS — •Sandra Gottwals[1], Andreas Müller[2], and Georg Schmidt[1,3] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Fachgruppe Nanostrukturierte Materialien, Halle — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Abteilung Elektronik, Halle — [3]Martin-Luther-Universität Halle-Wittenberg, Interdisziplinäres Zentrum für Materialwissenschaften, Halle

We want to use Nb-based micro-SQUIDS [1] to measure the Spin-Nernst-effect [2]. For this purpose we need to read out the SQUIDS with high resolution and keep current induced heating as low as possible. We have developed a new electronics setup for readout which is based on two separate digital-to-analog converters (DACs) running at high speed but with different scaling. The first converter is used to run a current ramp which gives a course measurement of the critical current. In a second measurement the second DAC creates a ramp close to the critical current at very high resolution. Once the critical current is established this way it can be measured using a high resolution voltmeter or analog-to-digital converter. The dual setup allows to automatically detect a wide range of critical currents, and immediate

shut-down when critical current is reached while at the same time giving a high resolution reading. The resolution is mainly determined by the final read-out device rather than by the resolution of the DACs.

[1] Wernsdorfer, Supercond. Sci. Technol. 22 (2009)
[2] Cheng, et. al., Phys. Rev. B 78 (2008)

TT 55.7 Wed 15:00 P2-OG3

Broadband acoustic measurements on the metallic glass $Zr_{59}Ti_3Cu_{20}Ni_8Al_{10}$ — •Alexander Prieschl, Sebastian Eisenhardt, Markus Döttling, Saskia Meissner, Arnold Seiler, and Georg Weiss — Physikalisches Institut, KIT Karlsruhe

Atomic two-level tunneling systems (TS) dominate the properties of disordered solids at low temperatures. While the standard tunneling model successfully describes thermodynamic properties of insulating glasses, it fails to predict the elastic properties of metallic glasses correctly. To explore the influence of conduction electrons on the density of states and the dynamics of TS ultrasonic experiments are performed. In superconducting glasses the interaction can be switched on and off by means of a magnetic field which suppresses superconductivity and therefore enables electrons to interact with TS.

Here we present measurements of the internal friction and the sound velocity of the superconducting bulk metallic glass $Zr_{59}Ti_3Cu_{20}Ni_8Al_{10}$ from 10 mK to room temperature. Low frequency acoustic measurements at 1 kHz are performed by using the vibrating reed technique, whereas frequencies up to 2 GHz are obtained by thin film piezoelectric transducers.

TT 55.8 Wed 15:00 P2-OG3

Superconducting qubit as a detector of atomic tunneling systems toggling on time scales spanning six orders of magnitude — •Saskia Meissner, Arnold Seiler, Jürgen Lisenfeld, Alexey V. Ustinov, and Georg Weiss — Physikalisches Institut, Karlsruher Institut für Technologie

AlO_x is a common material used for the production of Josephson junctions in superconducting qubits. It is known that the mostly disordered thin-film AlO_x contains atomic tunneling systems. Coherent tunneling systems couple strongly with their electric dipole moment to the qubit, giving rise to level repulsion in its spectrum. Slowly fluctuating tunneling systems are also observable if they are located close to the coherent ones and cause a local distortion of their potentials. Thus they are visible by telegraphic noise of the energy splitting of the coherent tunneling systems which can be measured on time scales from hours to minutes. The high-resolution single-photon spectroscopy measurement protocoll for the detection of coherent tunneling systems also allows us to determine fluctuation rates on a time scale of milliseconds by a special statistical analysis of the measured qubit states.

TT 55.9 Wed 15:00 P2-OG3

Coherence properties of superconducting qubits in large in-plane magnetic fields — •Andre Schneider, Jochen Braumüller, Marco Pfirrmann, Alexey V. Ustinov, and Martin Weides — Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

We intend to directly interface thin film ferromagnets with planar superconducting qubits to study the quantum dynamics within the magnet. To achieve this, superconducting qubits have to be placed in or close to a strong static magnetic field.

As a first step, we experimentally study the coherence properties of superconducting qubits under the influence of an external magnetic field which is oriented in parallel to the plane of the chip. The qubit is a superconducting concentric transmon having a microstrip geometry [1] showing up to 10 μs coherence times T1 and T2 at zero magnetic field. Qubit properties such as relaxation and dephasing times, as well as flux noise, are measured in an external field up to the mT range at temperatures below 50 mK.

[1] Braumüller *et al.*, APL **108**, 032601 (2016)

TT 55.10 Wed 15:00 P2-OG3

Investigation of a Josephson junction based parametric amplifier — •Patrick Winkel[1], Ivan Takmakov[2,3], Alexandre Karpov[3], Ivan Khrapach[2,3], Martin Weides[1,4], and Alexey V. Ustinov[1,3] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Moscow Institute of Physics and Technology, Moscow, Russia — [3]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia — [4]Material Science in Mainz, Johannes Gutenberg-University Mainz, 55128 Mainz, Germany

We design, fabricate and experimentally investigate a parametric amplifier based on the nonlinear inductance of Josephson junctions embedded into a superconducting resonator. The conventional design is based on a strongly coupled coplanar waveguide quarter-wave resonator terminated by a single SQUID. The weakly non-linear resonator is driven close to a bistable state where the system's response is highly sensitive to small perturbations. We performed four-wave-mixing experiments and obtained signal gain of up to 20 dB. The measured device performance is compared with theoretical expectations.

TT 55.11 Wed 15:00 P2-OG3

Electric transport and noise properties of Nb-HfTi-Nb Josephson Junctions — •Julian Linek[1], Benedikt Müller[1], Viacheslav Morosh[2], Thomas Weimann[2], Oliver Kieler[2], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Germany — [2]Fachbereich Quantenelektronik, Physikalisch-Technische Bundesanstalt, Braunschweig, Germany.

Nb-HfTi-Nb based superconductor-normal metal-superconductor (SNS) Josephson junctions offer high critical current density ($> 10^5$ A/cm^2) and non hysteretic current-voltage characteristics, which makes them highly suitable for their use in strongly miniaturized nanoSQUIDs. The high sensitivity of nanoSQUIDs can e.g. be used to detect the magnetization reversal of individual magnetic nanoparticles. To optimize the sensitivity of the devices and for increasing the range of operation temperature and magnetic field, a detailed understanding of the properties of the Nb-HfTi-Nb junctions as a function of their size and operation temperature is essential. Here we present an experimental study of the electrical transport and noise properties of single Nb-HfTi-Nb junctions. In particular, we have investigated the scaling of the resistance, critical current and noise level of the junctions with temperature (down to 300 mK) and junction size (down to $\sim$ 100 nm). Simulations of the current-voltage characteristics based on the RCSJ model have been compared to the experimental results, to check whether this model is appropriate for the description of these SNS Josephson Junctions.

TT 55.12 Wed 15:00 P2-OG3

Development of Nb nanoSQUIDs based on SNS junctions for operation in high magnetic fields — •Viacheslav Morosh[1], Benedikt Müller[2], Julian Linek[2], Maria Jose Martinez-Perez[2], Oliver Kieler[1], Thomas Weimann[1], Jörn Beyer[3], Thomas Schurig[3], Alexander Zorin[1], Reinhold Kleiner[2], and Dieter Koelle[2] — [1]Fachbereich Quantenelektronik, Physikalisch-Technische Bundesanstalt (PTB), Braunschweig — [2]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen — [3]Fachbereich Kryophysik und Spektrometrie, Physikalisch-Technische Bundesanstalt (PTB), Berlin

DC nanoSQUIDs (nSQs) with overdamped SNS sandwich-type (Nb/HfTi/Nb) Josephson junctions (JJ) developed for the investigation of small spin systems will be presented. Our smallest nSQs have JJ with linear dimensions $\leq$ 100 nm, effective loop areas $< 0.03\,\mu$m^2 and a distance between the JJ of $\sim$ 30 nm. Nb feeding strip lines of width $\sim$ 100 nm and thicknesses 160 nm/200 nm have been realized. Due to narrow line widths these nSQs show stable operation in external magnetic fields at least up to $\pm$0.25 T, which allows manipulating the spins of investigated objects over a wide field range. A magnetic moment sensitivity of a few tens of $\mu_B/\mathrm{Hz}^{1/2}$ has been demonstrated. Results achieved with different nSQ geometries and for single sub-μm JJ up to very high critical current densities ~ 1 MA/cm^2 will be presented. The noise properties including voltage noise of single JJ and flux noise of nSQs will be discussed.

This work was supported by the DFG (KI 698/3-1, KO 1303/12-1, SCHU 1950/5-1).

TT 55.13 Wed 15:00 P2-OG3

$YBa_2Cu_3O_7$ nanoSQUIDs for scanning SQUID microscopy — •Katja Wurster, Benedikt Müller, Jianxin Lin, Reinhold Kleiner, and Dieter Koelle — Physikalisches Institut and Center for Quantum Science (CQ) in LISA+, Universität Tübingen, Germany

The minuaturization of SQUID structures down to the sub-micron scale (nanoSQUIDs) is highly promising for their application in high-resolution scanning SQUID microscopy (SSM). Following recent achievements with nanoSQUIDs from conventional metallic superconductors, we are developing nanoSQUIDs based on the cuprate superconductor $YBa_2Cu_3O_7$ (YBCO) for SSM. We present here our efforts to develop YBCO nanoSQUIDs based on grain boundary Josepshon

junctions, grown on bicrystal $SrTiO_3$ substrates. These SQUIDs have to be fabricated on structures wich are suitable for implementation of their use in SSM. This includes in particular the development of structures which allow for the approach of the YBCO nanoSQUIDs to very small distances from the sample surfaces to be investigated. The use of YBCO offers operation over a wide range of temperature and magnetic field, which can significantly enhance the range of application of nanoSQUIDs for SSM-based nanoscale magnetic sensing and thermometry.

Technical support by R. Löffler and M. Turad from LISA$^+$ is gratefully acknowledged.

TT 55.14 Wed 15:00 P2-OG3

$YBa_2Cu_3O_7$ nanoSQUIDs for the investigation of single magnetic nanoparticles over a wide range of temperature and magnetic field — •Dennis Schwebius[1], Benedikt Müller[1], Maria José Martínez-Pérez[1], Jianxin Lin[1], Dana Korinski[1], Reinhold Kleiner[1], Javier Sesé[2], and Dieter Koelle[1] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Germany — [2]Laboratorio de Microscopías Avanzadas (LMA), Instituto de Nanociencia de Aragón (INA), Universidad de Zaragoza, Spain

NanoSQUIDs based on the cuprate superconductor $YBa_2Cu_3O_7$ (YBCO) are promising devices for the investigation of single magnetic nanoparticles (MNPs), as they offer high spin sensitivity down to a few Bohr magnetons/$\sqrt{\text{Hz}}$, combined with the possibility to operate them over a wide range of temperature (up to $\sim 80\,\text{K}$) and magnetic field (up to the Tesla range). Here, we present our efforts to optimize the performance and reliable operation of YBCO nanoSQUIDs, based on grain boundary Josephson junctions, in strong magnetic fields applied in the plane of the SQUID loop and perpendicular to the grain boundary plane. Special care has to be taken on the precise alignment of the external magnetic field. Moreover, we present first results on the characterization of the magnetic properties of Co MNPs, grown by focused electron beam induced depostion directly on top of the SQUID loops, demonstrating the feasibility of using YBCO nanoSQUIDs for single MNP measurements.

TT 55.15 Wed 15:00 P2-OG3

Emission of terahertz radiation from intrinsic Josephson junctions in $Bi_2Sr_2CaCu_2O_{8+x}$ stacks — •Johannes Hampp[1], Olcay Kizilaslan[1,2], Raphael Wieland[1], Fabian Rudau[1], Xianjing Zhou[3,4], Min Ji[3,4], Ya Huang[3,4], Luyao Hao[3,4], Nickolay Kinev[5], Oleg Kiselev[5], Peiheng Wu[3], Valery Koshelets[5], Huabing Wang[3,4], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Germany — [2]Inonu University, Department of Biomedical Engineering, Faculty of Engineering 44280, Malatya, Turkey — [3]National Institute for Materials Science, Tsukuba, Japan — [4]Research Institute of Superconductor Electronics, Nanjing University, China — [5]Kotel'nikov Institute of Radio Engineering and Electronics, Moscow, Russia

Josephson junctions (JJs) offer a natural way to convert a dc-voltage into high-frequency electromagnetic radiation. The high-T_c superconductor $Bi_2Sr_2CaCu_2O_{8+x}$ intrinsically forms stacks of JJs. Such stacks can be used as generators for electromagnetic radiation of frequencies in the sub-THz and low-THz regime. Radiation power and frequency strongly depend on the electric and thermal parameters of the stack. To systematically investigate this dependence we vary these parameters in-situ by changing the charge carrier density via current injection. Experimental results and theoretical simulations will be presented.

TT 55.16 Wed 15:00 P2-OG3

On quantum features of a driven swept-bias Josephson junction — •Harald Losert[1], Karl Vogel[1], Benjamin Neumeier[2], Rosina Menditto[2], Edward Goldobin[2], Dieter Kölle[2], Reinhold Kleiner[2], and Wolfgang P. Schleich[1,3] — [1]Institut für Quantenphysik, Universität Ulm, D-89069 Ulm, Germany — [2]Physikalisches Institut, Universität Tübingen, D-72076 Tübingen, Germany — [3]Texas A&M University, College Station, TX 77843

Josephson junctions are a well-known model system for the observation of quantum tunneling. The phase difference in a current-biased junction behaves like the position of a particle in a tilted washboard potential. The escape of this phase-particle corresponds to the voltage switching of the associated junction.
The escape from the potential can be explained quantum mechanically by tunneling from the ground state, or an excited state. However, in the presence of a periodic driving field, it has been shown [1][2], that even classical calculations reproduce the experimental data for quantum mechanical key features, e.g. Rabi oscillations.
Resuming this discussion, we focus on Josephson junctions with large critical currents and consider a swept-bias experimental setup. We compare the switching current distributions of our recent experiments with numerical results for both quantum mechanical as well as classical time evolution.

[1] Marchese *et al.*, *Eur. Phys. J. Special Topics* **147**, 333 (2007)
[2] Blackburn *et al.*, *Phys. Rev. B* **85**, 104501 (2012)

TT 55.17 Wed 15:00 P2-OG3

Current contributions in a superconducting SET due to Josephson transport — •Susanne Sprenger, Thomas Lorenz, and Elke Scheer — Universität Konstanz, 78467 Konstanz, Deutschland

When measuring superconducting transport trough two tunnel junction separating a small island from the leads, Coulomb blockade effects can be observed. Using orthodox theory [1, 2] one can identify the contributions to the current through this all superconducting single electron transistor (SSET).

We investigate a SSET formed by one oxide barrier and one mechanically controllable break junction (MCBJ). We present measurements on samples, differing in the transparency of the oxide barrier, either allowing only tunneling or in addition Josephson transport, whereas the MCBJ is broken to form a mere tunnel contact. In the Josephson regime additional contributions to the current in the superconducting gap can be observed, giving first evidence for coherent transport. The measurements are compared with the predictions of orthodox theory.

[1] K. K. Likharev, Proc. IEEE 87, 606 (1999)
[2] R. J. Fitzgerald, Phys. Rev. B 57, R11073(R) (1997)

TT 55.18 Wed 15:00 P2-OG3

MOCCA: A 4k-pixel molecule camera for the position and energy resolving detection of neutral molecule fragments at the Cryogenic Storage Ring CSR — •S. Allgeier[1], C. Enss[1], A. Fleischmann[1], L. Gamer[1], L. Gastaldo[1], S. Kempf[1], C. Krantz[2], O. Novotný[2], D. Schulz[1], and A. Wolf[2] — [1]Heidelberg University — [2]MPIK Heidelberg

The Cryogenic Storage Ring CSR at the Max Planck Institute for Nuclear Physics in Heidelberg is designed to prepare and store molecular ions in their rotational and vibrational ground states. A key requirement for the study of electron-ion interactions within CSR is the identification of reaction products. The use of metallic magnetic calorimeters (MMCs) allows for identifying all neutral products since the deposited kinetic energy of incident particles into MMC absorbers can be used as a measure of the particle mass. To actually resolve the full reaction kinematics, a position sensitive coincident detection of multiple reaction products is necessary.

For these measurements we designed MOCCA, a 4k-pixel molecule camera based on MMCs with a detection area of 45 mm×45 mm, which is segmented into 64×64 absorbers and read out using only 32 SQUIDs. We discuss the detector design and its microfabrication as well as its multi-hit capability, cross-talk and expected energy resolution for photons and massive particles. In addition, we outline our plans for integrating MOCCA and its ^{3}He/^{4}He dilution refrigerator into CSR.

TT 55.19 Wed 15:00 P2-OG3

dc-SQUIDs for readout of metallic magnetic calorimeters — •Daniel Richter, Felix Herrmann, Anna Ferring, Andreas Fleischmann, Loredana Gastaldo, Sebastian Kempf, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

Two-stage current-sensing dc-SQUIDs are presently the devices of choice to read out single-channel metallic magnetic calorimeters (MMCs). However, it is well known that parasitic inductances in the input circuitry lead to a reduction of the detecor signal size and that SQUID noise can cause a significant contribution to the energy resolution. In addition, parasitic mutual inductances between the input and feedback coil degrade the detector performance. In order to minimize these effects, we are currently developing two-stage current-sensing dc-SQUIDs that are optimized for MMC readout.

We discuss our different SQUID designs including single SQUIDs forming the front-end to the detector as well as N-SQUID series arrays providing signal amplification for the front-end SQUID at low temperatures. Our front-end SQUIDs are second-order parallel gradiometers,

have an input coil inductance of about 1 nH and show a particularly small parasitic coupling between the input and feedback coil. Our N-SQUID series arrays provide an on-chip bias resistor and include all circuitry that is required for easily building two-stage SQUID setups. We will show that our two-stage SQUID setups exhibit a very good noise performance reaching values down to the quantum limit. This makes it ideally suited for readout of high-resolution MMCs.

TT 55.20 Wed 15:00 P2-OG3

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

Metallic magnetic calorimeters (MMC's) are energy dispersive particle detectors operated below 100 mK which excel in energy resolution, dynamic range and linearity. They use a paramagnetic temperature sensor to convert the energy deposited by means of photon absorption into a magnetic flux change in a SQUID, which is 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 micro-fabrication techniques, while lowering the readout noise close to quantum limit. The combination of both rewarded us with a world record instrumental linewidth of 1.6 eV (FWHM) for 6 keV X-rays, measured with our maXs-20 detector, a 1x8 pixel array. We summerize the physics of MMCs focusing on solid state effects, we present application-oriented microfabrication processes and cryogenic setups and we show recent results of our X-ray detectors. This includes the maXs-30 detector, an 8x8 pixel array optimized for X-rays up to 30 keV and a new design, which places the temperature sensor directly in a SQUID for maximized signal coupling with an expected instrumental linewidth below 1 eV (FWHM) for X-rays up to 10 keV. Our detectors are operated in a cryogen free 3He/4He-dilution refrigerator at the tip of a 40 cm long cold finger at $T = 20$ mK.

TT 55.21 Wed 15:00 P2-OG3

Polar-maXs: Micro-calorimeter based X-ray polarimeters — •Christian Schötz[1], Daniel Hengstler[1], Jeschua Geist[1], Sebastian Kempf[1], Loredana Gastaldo[1], Andreas Fleischmann[1], Christian Enss[1], and Thomas Stöhlker[2,3,4] — [1]KIP, Heidelberg University — [2]Helmholtz-Institute Jena — [3]GSI Darmstadt — [4]IOQ, Jena University

We are presently developing the x-ray detector system Polar-maXs, which will combine for the first time the high energy resolution, large dynamic range and excellent linearity of magnetic micro-calorimeters with the sensitivity to polarization caused by polarization-dependent Compton or Rayleigh scattering in an array of scatterers.

Polar-maXs consists of two layers. The first layer comprises a 4 x 4 array of x-ray scatterers behind a corresponding array of collimator holes. Depending on the energy range of interest and whether Compton or Rayleigh scattering is to be used, these scatterers are fabricated from low-Z or high-Z material. The scattered x-rays are detected by an array of 576 x-ray absorbers read-out by paramagnetic temperature sensors as metallic magnetic micro-calorimeters (MMC). Each absorber covers an area of 0.5mm x 0.5mm and is made of 10 micrometer thick gold, to guarantee high stopping power for x-ray with energies up to 20 keV and an energy resolution of better than 20eV (FWHM) in the complete energy range. We discuss general design considerations as well as the results of Monte-Carlo simulations for a variety of detector designs. We present the results of first measurements with the Hydra-principle.

TT 55.22 Wed 15:00 P2-OG3

Superconducting nanowire single-photon detectors with multi-photon resolution for integrated quantum photonics on GaAs — •Eric-René Reutter[1,2], Ekkehart Schmidt[1], Mario Schwartz[3], Hannes Rotzinger[2], Konstantin Ilin[1], Michael Jetter[3], Peter Michler[3], Alexey V. Ustinov[2], and Michael Siegel[1] — [1]Institut für Mikro- und Nanoelektronische Systeme (IMS), Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Physikalisches Institut (PHI), Karlsruher Institut für Technologie, Karlsruhe, Germany — [3]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Universität Stuttgart, Stuttgart, Germany

Integrated quantum photonic devices are one of the most promising fields for future information processing technologies. Superconducting nanowire single-photon detectors (SNSPDs) can function as the perfect on-chip detection part, with low dark count and high event count rates, as well as picosecond timing resolution, high detection efficiency and excellent scalability. Their drawback is not having intrinsic energy and photon-number resolution (PNR). Quasi-PNR can be achieved using multi-pixel arrays in which SNSPDs are parallel shunted by resistors [1]. We have demonstrated quasi-PNR functionality of SNSPDs made of 4.9 nm thick and 100 nm wide NbN nanowires on GaAs. The detectors were shunted by 50-60 Ω palladium resistors forming 4-pixel arrays. We investigated multi-photon resolution capability of such detectors being excited by a fs-pulse NIR laser. Details on the dependence of the detector response on light intensity will be presented and discussed.

[1] S. Jahanmirinejad *et al.*, Opt. Express **20** 2012, 5017-5028

TT 56: Poster Session: Low-Dimensional Systems

Time: Wednesday 15:00–19:00 Location: P2-OG4

TT 56.1 Wed 15:00 P2-OG4

Oxidation and temperature dependent resistivity of VSe_2 flakes — •Benedikt Brechtken, Christopher Belke, Hennrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover

Many 2D materials are of interest for the design of innovative devices. But some of them are chemically less stable than the well known graphene. The influence on the properties of VSe_2 flakes through oxidation in ambient air at room temperature is studied. Therefore VSe_2 flakes were fabricated with the scotch tape method under nitrogen atmosphere and Cr/Au-contacts were build on the flakes with e-beam lithography.

The surface oxidation was investigated via optical microscopy and atomic force microscopy. A slow oxidation and formation of small oxidhills on the flake surface could be observed. A two point measurement at room temperatur showed a resistance of 250 Ohm for a 30 nm thick flake.

Furthermore the temperature dependence of the resistivity was studied in a He cryostat. Between room temperature and the Debye temperature a linear dependance was measured. Under the Debye temperature the dependance showed a power-law relation. That is a classical metallic behavior as it was found in VSe_2 bulk material [1]. Around 95 K a charge-density-wave was expected [2]. That could not be measured, most likely because of the low mobility of the sample.

[1] A. Toriumi, and S. Tanaka, Physika **105B**, 141, (1981)

[2] J. Yang, et al., Applied Physics Letters **105**,063109 (2014)

TT 56.2 Wed 15:00 P2-OG4

Photoemission study of the bulk band dispersion in 1T-TaS_2 at 30 K — •Arlette S. Ngankeu[1], Sanjoy K. Mahatha[1], Marco Bianchi[1], Charlotte E. Sanders[1], Kai Rossnagel[2], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark — [2]Institute for Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany

The ground states of many layered transition metal dichalcogenides, including 1T-TaS_2, are governed by charge density waves (CDWs) associated with periodic lattice distortions. These distortions are accompanied by changes of the electronic structure due to Brillouin zone reconstructions. In the case of 1T-TaS_2, the low-temperature commensurate CDW state even coexists with a Mott-insulating ground state. While many studies have addressed the origin of the CDW in 1T-TaS_2, there have been recent theoretical results specifically addressing the three-dimensional nature of the bands associated with the Mott state, finding that the Mott state leads to an insulating in-plane state while the out-of-plane dispersion of the state remains metallic.

We have investigated the electronic band structure of 1T-TaS_2 in the commensurate-CDW phase in all three dimensions by means of synchrotron radiation-based angle resolved photoemission spectroscopy. The measured in-plane band structure is consistent with previous results from the literature. We observe an out-of-plane dispersion of the lower Mott state, as predicted, but no Fermi crossing, such that a 3D

insulating behavior is retained.

TT 56.3 Wed 15:00 P2-OG4

Charge and orbital order in 1T-TaS_2 — •Florian Heinsch[1,2], Helmuth Berger[3], Bernd Büchner[4], Thomas Cowan[1], Michal Dušek[5], Tobias Förster[1], Joachim Wosnitza[1], Klaus Koepernik[4], Václav Petříček[5], Tobias Ritschel[2], Marc Uhlarz[1], and Jochen Geck[2] — [1]HZDR — [2]TU Dresden — [3]EPFL — [4]IFW Dresden — [5]Institute of Physics, Prague

Recently discovered phenomena in thin films of 1T-TaS_2, like a laser induced ultra-fast switching to a hidden quantum states, offer great potential for future applications and prove that one has not yet unraveled the microscopic interactions behind the origin of the electronic order in this system completely [1].

One piece of the puzzle seems to be an orbital texture that is intertwined with the CDW in the commensurate state [2]. We investigated the incommensurate structural modulations of 1T-TaS_2, which occur above T=350K, by means of single crystal X-ray diffraction and refined the crystal structure in the formalism of a (3+2)-dimensional superspace. Based on these information, we performed DFT calculations for repeating clusters. The obtained highest occupied molecular orbitals imply an orbital ordering. Since those degrees of freedom are expected to affect the magnetic susceptibility as well, we also started to reinvestigate the magnetic field dependence of the CDW-instability in 1T-TaS_2. For the future we aim on time-resolved diffration experiments in high magnetic fields to gain insights into microscopical interactions.

[1] L. Stojchevska et al., Science 344.6180 (2014), pp. 177-180
[2] T. Ritschel et al., Nature Physics 11.4 (2015), pp. 328-331

TT 56.4 Wed 15:00 P2-OG4

Low energy dynamics in charge ordered $R_{0.5}Sr_{0.5}MnO_3$ (R = Nd and Pr) manganite thin films — •Rakesh Rana[1], Johannes Schmidt[1,2], Jörg Grenzer[1], Harald Schneider[1], Manfred Helm[1,2], and Alexej Pashkin[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany

Transition metal oxides exhibit complex interplay between the spin, charge, orbital and lattice degrees of freedom which may result in colossal magnetoresistance, superconductivity; charge ordered (CO) phases, etc. The half-doped $Pr_{0.5}Sr_{0.5}MnO_3$ manganite represents a unique stripe type CO-orbital order that induces transport and magnetic anisotropy whereas the CO in $Nd_{0.5}Sr_{0.5}MnO_3$ is charge-exchange (CE)-type which is isotropic in nature.

Epitaxial manganite thin films with a thickness of 200nm were grown on (100), (110), and (111) oriented $(LaAlO_3)_{0.3}(Sr_2TaAlO_6)_{0.7}$ substrates by pulsed laser deposition technique. Terahertz (THz) time-domain spectroscopic data reveal charge density wave (CDW) resonance centered around 5-6 meV for (110) oriented films and Drude-like conductivity for (100) and (111) oriented films. The CDW resonance frequency can be tuned from 4 meV to 6 meV for (110) oriented films and corroborate well with the magnetization measurements. The nonlinear conductivity related to the sliding of the pinned CDW character makes the studied systems promising candidates for ultrafast coherent control of charge transport by resonant THz pumping.

TT 56.5 Wed 15:00 P2-OG4

Correlation length in topological insulators: how different are a mug and a donut? — •Wei Chen, Markus Legner, Andreas Rüegg, and Manfred Sigrist — ETH Zurich, Zurich, Switzerland

We all know that a mug and a donut have the same topology. But how different are they? How different are two topological insulators that have the same topological invariant? We show that the correlation function that characterizes the topological insulators in 1D is a charge polarization correlation between Wannier states, and in 2D it is an itinerant circulation correlation between Wannier states. Suprisingly, these Wannier state correlation functions are nonzero in both topologically trivial and nontrivial states. The correlation function allows to extract a correlation length that characterizes the difference between topological insulators that are close to those that are far away from the topological phase transitions. The critical exponent of correlation length further suggests the existence of universality classes.

TT 56.6 Wed 15:00 P2-OG4

Mixed singlet-triplet and possible topological superconductivity in hole doped Sr_2IrO_4 — Mohammad-Hossein Zare[1], •Mehdi Biderang[2], and Alireza Akbari[2] — [1]Department of Physics, Qom University of Technology, Qom, Iran — [2]Asia Pacific Center for Theoretical Physics, POSTECH, Pohang, Korea

We investigate the potential existence of a superconducting phase in hole doped Sr_2IrO_4. Based on the mean field calculations, a mixed singlet-triplet superconductivity due to spin-orbit coupling has been found. Our calculation on a nanoribbon geometry shows possible existence of the topologically peotected edge states while the spin-triplet gap is larger than the spin-singlet one. Finally, we propose an innovative route for experimental observation of the edge states based on the quasiparticle interference (QPI) pattern.

TT 56.7 Wed 15:00 P2-OG4

Edge states at zigzag edges of Bi honeycomb bilayers on Nb(110) — •Fang Yang[1], Jasmin Jandke[1], Tim Storbeck[1], Timofey Balashov[1], Anuva Aishwarya[2], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Wolfgang-Gaede Str. 1, 76131 Karlsruhe, Germany — [2]Indian Insitute of Science, Bangalore, India

Islands of Bi showing (110)- and (111)-orientated facets were grown on Nb(110) and were studied with STM at low temperatures. On the (111) facets, both bilayer steps of zig-zag termination display topological edge states in contrast to that of single bilayer step-edges on bulk Bi. This is evidenced by locally resolved density-of-states near the edges revealing the characteristic distribution of edge states, i.e. dangling bond states and bulk-derived topological edge states. Further, we investigated the charge distribution of the surface state electrons on the Bi(110) surface. We find that the electronic states are highly anisotropic within the unit cell forming one dimensional stripes. Our findings indicate a causal link between the Bi(111) edge states and Bi(110) surface states as they are both related to the zig-zag termination of the honeycomb structure of Bi.

TT 56.8 Wed 15:00 P2-OG4

Topological charge pumping due to rotating magnetic fields in a Rashba spin-orbit coupled curved nanowire — •Sudhakar Pandey[1], Paola Gentile[2], Mario Cuoco[2], and Carmine Ortix[1,3] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, 01069 Dresden, Germany — [2]CNR-SPIN and Dipartimento di Fisica "E. R. Caianiello", Universita di Salerno, I-84084 Fisciano (Salerno), Italy — [3]Institute for Theoretical Physics, Center for Extreme Matter and Emergent Phenomena, Utrecht University, Princetonplein 5, 3584 CC Utrecht, Netherlands

Topological charge pumping refers to transport of charge in a system due to an adiabatic temporal change in the periodic potential. The transported charge per pump cycle is quantized, and purely determined by the topology of the pump cycle, which can be characterized by a topological invariant: the Chern number. Although introduced originally more that three decades ago [1], its experimental realization has been achieved recently in ultracold bosonic [2] and fermionic [3] atoms loaded in the optical superlattices. In this work we demonstrate that a Rashba spin-orbit coupled curved wire subject to a rotating magnetic field can work as a topological charge pump. In a descretized system with N atoms per unit cell we find a Chern number C=2 at the band fillings n=1/N and (N-1)/N. The fact that these results are robust even in the continuum limit makes our proposal feasible experimentally.

[1] D.J. Thouless, Phys. Rev. B 27, 6083 (1983)
[2] M. Lohse et al., Nat. Phys. 12, 350 (2016)
[3] S. Nakajima et al., Nat. Phys. 12, 296 (2016)

TT 56.9 Wed 15:00 P2-OG4

Exact Tensor Network States for the Kitaev Honeycomb Model — •Philipp Schmoll and Román Orús — Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany

The spin-1/2 Kitaev honeycomb model was originally proposed in the context of topological quantum computation. This analytically solvable model realizes a spin liquid and exhibits rich physical behaviour, such as abelian and non-abelian anyons as excitations. Our aim is to describe the eigenstates of the model using tensor network methods, which offer efficient descriptions of quantum many-body systems. In particular we exploit parity preservation and build a fermionic tensor network to express the eigenstates of the Hamiltonian in the ground-state vortex sector. We implement the network for small lattices with periodic boundary conditions in order to verify the approach for the model in the thermodynamic limit.

TT 56.10 Wed 15:00 P2-OG4

Thickness dependent electronic and structural transition in $BaBiO_3$ thin films on $SrTiO_3$ — •Michael Zapf, Sebastian Elsässer, Martin Stübinger, Jean Geurts, Michael Sing, and Ralph Claessen — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany

$BaBiO_3$ (BBO), the parent material of the high-T_C superconductor $Ba_{1-x}K_xBiO_3$ (T_C=30 K), has recently been proposed to be a large gap topological insulator, when heavily n-doped. This state may be accessed experimentally by electric gating and doping of BBO thin films as single or multilayer structures.

To investigate, as a first step, the properties of pristine BBO in the thin film limit, we have grown a series of BBO films of various thicknesses on $SrTiO_3$ with pulsed laser deposition (PLD). We found significant modulations of the structural and electronic characteristics of the films. Raman spectroscopy indicates a reduction of the lattice symmetry from a cubic to a distorted perovskite lattice as in bulk-like BBO at a thickness of a few unit cells. Beyond this thickness, photoemission valence band spectra of the thin films resemble the spectral shape known from BBO single crystals. Further photoemission measurements show that this structural and electronic crossover is determined by significant stoichiometry deviations occurring at the beginning of BBO deposition.

TT 56.11 Wed 15:00 P2-OG4

Interface band engineering in $LaAlO_3/SrTiO_3$ heterostructures — •Judith Gabel[1], Philipp Scheiderer[1], Michael Zapf[1], Martin Stübinger[1], Christoph Schlueter[2], Tien-Lin Lee[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — [2]Diamond Light Source Ltd., Didcot, United Kingdom

Novel two-dimensional electron systems at the interfaces of oxide heterostructures, as e.g. at the $LaAlO_3/SrTiO_3$ (LAO/STO) heterointerface, recently have attracted much attention. A key requirement for future applications is the controllability of the electronic interface properties. We show that these properties can be controlled in LAO/STO by the oxygen vacancy (V_O) concentration which can in turn be adjusted during photoemission experiments by means of synchrotron light irradiation and simultaneous oxygen dosing. In detail, the V_O concentration determines the density of mobile and trapped charge carriers as well as the band bending and alignment at the interface. We systematically investigate these properties on (001) and (111) oriented LAO/STO heterostructures with controlled V_O concentrations by depth profiling the film and substrate core levels by means of angle-dependent hard X-ray photoelectron spectroscopy, while resonant soft X-ray photoemission is used to probe the interfacial valence band states.

TT 56.12 Wed 15:00 P2-OG4

Emergence of interfacial conductivity in the $LaAlO_3$ capped $LaVO_3/SrTiO_3$ heterostructure — •Martin Stübinger, Judith Gabel, Philipp Gagel, Michael Sing, and Ralph Claessen — Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), 97074 Würzburg, Germany

Akin to the well known oxide heterostructure $LaAlO_3/SrTiO_3$ (LAO/STO) a conducting interface is found also between the strongly correlated, polar Mott insulator $LaV^{3+}O_3$ (LVO) and the non-polar band insulator STO. Since $LaV^{3+}O_3$ tends to overoxidize to the thermodynamically more stable $LaV^{5+}O_4$ phase when exposed to air, a suitable passivation is required. Therefore, we have employed pulsed laser deposition thin film growth of LVO films with a crystalline LAO capping layer. *In situ* photoemission measurements of samples before and after being exposed to air show that the V oxidation state can indeed be stabilized by the LAO capping layer. By transport measurements, we identify an insulator-to-metal transition at a combined LAO/LVO overlayer thickness of 4 unit cells. The metallicity holds for different combinations of LAO and LVO thickness as long as the total overlayer thickness is 4 uc or higher. Thus, both LAO and LVO play a cooperative role in inducing interfacial conductivity in this system. We discuss these findings in terms of an interplay of the polar nature of LAO and LVO and defect states that provide mobile charge carriers.

TT 56.13 Wed 15:00 P2-OG4

Tuning the electric interface properties of amorphous $AlO_x/SrTiO_3$ interfaces — •Berengar Leikert, Judith Gabel, Michael Sing, and Ralph Claessen — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany

Two dimensional electron systems (2DESs) at the interfaces of oxide heterostructures are considered a promising platform for future microelectronic technology which may utilize the rich electronic behavior emerging at the interfaces of transition metal oxides. A simple and cost-effective method to create a 2DES is to deposit Al on the surface of $SrTiO_3$. It reduces the first oxide layers and leads to an n-doping of the oxide surface. By changing the Al redox potential via growth in oxygen atmosphere we can tune the electronic interface properties, which are probed by x-ray photoelectron spectroscopy of the film as well as the substrate core levels. Complementary transport experiments yield information about charge carrier concentration and mobility which are also shown to depend on the Al redox potential. Comparing the results from spectroscopy to the transport measurements for samples with differing carrier mobility and concentration we gain a deeper understanding of the properties governing transport at transition metal oxide interfaces.

TT 56.14 Wed 15:00 P2-OG4

Probing the dimensionality-driven metal-insulator transition in spin-orbit coupled $SrIrO_3$ thin films — •Philipp Schütz[1], Lenart Dudy[1], Judith Gabel[1], Martin Stübinger[1], Marius-Adrian Husanu[2], Vladimir Strocov[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — [2]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland

Although typically viewed to be disparate properties, the large spin-orbit-coupling (SOC) and relatively weak electronic correlations are roughly of the same order of magnitude in iridate compounds. The prototypical Ruddlesden-Popper iridates $Sr_{n+1}Ir_nO_{3n+1}$ have attracted special attention since they exhibit a SOC-induced Mott transition dependent on the value of n. Whereas the quasi-two-dimensional compound Sr_2IrO_4 ($n = 1$) shows a Mott-like insulating state, its three-dimensional analogue $SrIrO_3$ ($n = \infty$) is a correlated metal in proximity to a metal-insulator-transition. As an alternative to single crystal growth of Ruddlesden-Popper-iridates with different n, we investigate the effect of dimensionality through synthesis of atomically thin $SrIrO_3$ films by pulsed laser deposition, which analogously exhibit a metal-insulator-transition as function of thickness. We present a systematic investigation of the k-resolved electronic structure near the metal-insulator-transition by means of synchrotron-based soft x-ray angular-resolved photoemission spectroscopy (SX-ARPES), which sheds light on the intricate interplay between spin-orbit coupling, electronic correlations and dimensionality.

TT 56.15 Wed 15:00 P2-OG4

Tuning electronic phases and topological properties in $3d$-oxide honeycomb lattices confined within the corundum structure — •Okan Köksal, Santu Baidya, and Rossitza Pentcheva — Fakultät für Physik and Center of Nanointegration (CENIDE), Universität Duisburg-Essen, 47057 Duisburg

Using density functional theory including an on-site Coulomb term, we explore electronic and possibly topologically nontrivial phases in $3d$ transition metal oxide honeycomb layers confined in the corundum structure (α-Al_2O_3) along the [0001] direction. Except for X=V, Cr and Fe, most of the systems exhibit a ground state that is distinct from the corresponding bulk X_2O_3 compound. In particular, ferromagnetic X=Ti, Mn, Ni and metastable Co exhibit a characteristic set of four bands with a Dirac crossing close to the Fermi level. Our results indicate that the Dirac point can be tuned to the Fermi level using strain. Switching on spin-orbit coupling, a finite anomalous Hall conductivity with values up to 0.75 e^2/h is obtained. Parallels to the perovskite analogons $LaXO_3/LaAlO_3(111)$ [1] are discussed.

Support by the DFG within priority program TRR80, project G3 and a computational grant at the Leibniz Rechenzentrum are gratefully acknowledged.

[1] D. Doennig, S. Baidya, W. E. Pickett, and R. Pentcheva, Phys. Rev. B **93**, 165145 (2016)

TT 56.16 Wed 15:00 P2-OG4

Magnetotransport properties of the organic superconductor κ-$(ET)_2Cu[N(CN)_2)]Cl$ near the Mott-insulating transition — •Sebastian Oberbauer[1,2], Michael Kunz[1], Werner Biberacher[1], Natalia D. Kushch[3], and Mark V. Kartsovnik[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Technische Universität München, Garching, Germany — [3]Institute of Problems of

Chemical Physics, Chernogolovka, Russia

κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$)]Cl belongs to the family of charge transfer salts and shows many interesting phenomena at low temperatures. Especially the existence of a superconducting phase at temperatures up to 12.8 K bordering a magnetically ordered Mott-insulating state are of big interest in current research. This metal-insulator transition (MIT) can be tuned by applying hydrostatic pressures $\leq$ 0.4 kbar. Together with its highly anisotropic conductivity, this makes the compound a model example of a quasi-two-dimensional correlated electronic system.

Here we report on a magnetotransport study of κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$)]Cl under pressure, in the vicinity of the MIT. A particular focus is put on tracing the behavior of Shubnikov - de Haas oscillations. While the oscillation frequencies only weakly change with pressure, the effective cyclotron masses exhibit a significant increase, accelerating towards the MIT. We compare the experimental data with those obtained on similar κ-type organic conductors and with theoretical predictions.

TT 56.17 Wed 15:00 P2-OG4

Transport and thermodynamic studies of the metal-insulator transition in κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl under He-gas pressure — •Caroline Delleske[1], David Zielke[1], Elena Gati[1], Harald Schubert[1], John A. Schlueter[2], and Michael Lang[1] — [1]Physikalisches Institut, SFB/TR49, Goethe Uni Frankfurt, DE — [2]Materials Science Division, NSF, Arlington, Virginia, USA

Organic charge-transfer salts show a wide variety of electronic phases resulting from strong electron correlations in low dimensions, such as superconductivity or multiferroicity. The members of the κ-(BEDT-TTF)$_2$X family are representing model systems to investigate the interplay of strong on-site and inter-site Coulomb repulsion in 2D. Here we focus on the less intensively studied system κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl [1, 2], showing a metal-insulator (MI) transition at $T_{MI} \approx 30$ K which has been assigned to charge-order [1]. We report on a detailed characterization of the material's low-temperature properties by transport and thermodynamic measurements at ambient pressure, as well as under finite He-gas pressure. We find a slightly broadened MI transition, consistent with literature [2], which can be rapidly suppressed with increasing pressure. Surprisingly, no indications for superconductivity can be found up to pressures of $p = 300$ MPa and temperatures down to $T = 2.4$ K. In addition, we will present thermodynamic studies of the specific heat and thermal expansion to unravel the role of spin and lattice degrees of freedom at T_{MI}.

[1] N. Drichko et al., PRB 89, 075133 (14)
[2] S. Yasin et al., Physica B 407, 1689 (12)

TT 56.18 Wed 15:00 P2-OG4

Pressure- and temperature-dependent optical investigations on α-(BEDT-TTF)2I3 — •Weiwu Li[1], Ece Uykur[2], Christine A. Kuntscher[2], Dieter Schweitzer[1], and Martin Dressel[1] — [1]1.Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]Experimentalphysik II, Universität Augsburg, 86135, Augsburg, Germany

The two-dimensional organic conductor α-(BEDT-TTF)2I3 exhibits a metal-insulator transition at Tco=135K with a charge-ordered ground state. This system is considered to host massless Dirac electrons under hydrostatic pressure as high as 1.5 GPa, which has been confirmed both theoretically and experimentally. For better understanding of the charge dynamics in the Dirac state, pressure-dependent infrared measurements have been performed previously. Unfortunately, limited by a maximum pressure of 1 GPa, no final evidence of the Dirac electrons could be found. As an extension to the previous measurements, we performed reflectivity measurements under pressure (up to 4GPa) between 100 and 8000 cm-1 down to 6 K by using diamond anvil cell. As a result, with increasing pressure we observed a Drude component developed below 600 cm-1 at the expense of the suppression of the mid-infrared band. The charge order still exists up to 1.6 GPa, where the conductivity already shows metallic behavior. At the highest pressure (4 GPa), the optical conductivity shows almost no temperature dependence below 90 K with a Drude term below 500 cm-1 and a constant conductivity extends up to 1500 cm-1, which point out the coexistence of the massive charge carriers and the massless Dirac electrons.

TT 57: SYQO: Quantum Optics on the Nanoscale: From Fundamental Physics to Quantum Technologies (joint symposium HL,DS,O,TT, organized by HL)

Time: Thursday 9:30–12:30 Location: HSZ 02

Invited Talk TT 57.1 Thu 9:30 HSZ 02

Quantum dot based quantum technologies — •Pascale Senellart — CNRS - Université Paris-Saclay, 91460 Marcoussis, France

Scaling optical quantum technologies requires efficient single photon sources and two-photon gates. Such devices can be obtained using artificial atoms like semiconductor quantum dots (QDs). Yet, an ideal atom-photon interface is required, where the QD interacts with only one mode of the optical field and is free from decoherence. We have developed a near-optimal QD-photon interface by deterministically coupling a QD to a microcavity [1]. With an electrical control, the QD transition is shown to be almost decoherence free. The QD-cavity devices present a cooperativity of 12 and the QD state can be coherently manipulated with a π-pulse obtained for only 4 incident photons [2]. The devices operate as bright solid-state single-photon sources with single photon purity and indistinguishability above 98% and a brightness exceeding 20 times that of parametric down-conversion sources [3]. We also report on a single-photon filter that converts a coherent pulse into a highly non-classical light wavepacket [4], a first step toward deterministic two photon gates.

[1] A. Dousse, et al., Phys. Rev. Lett. 101, 267404 (2008). [2] V. Giesz, et al., Nature Communications 7, 11986 (2016). [3] N. Somaschi, et al., Nature Photonics 10, 340 (2016). [4] L. De Santis, et al., arXiv:1607.05977.

Invited Talk TT 57.2 Thu 10:00 HSZ 02

Controlled strong coupling of a single quantum dot to a plasmonic nanoresonator at room temperature — Heiko Gross[1], Joachim M. Hamm[2], Tommaso Tufarelli[2], Ortwin Hess[2], and •Bert Hecht[1] — [1]Nano-Optics and Biophotonics Group, Universität Würzburg, 97074 Würzburg, Germany — [2]The Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

We demonstrate controlled and tunable strong coupling of a mesoscopic plasmonic slit resonator and a single colloidal quantum dot at room temperature. Strong coupling is achieved (i) by placing the quantum dot within the mode field of the nanoresonator with nm precision using scanning probe technology and (ii) by exploiting the collective coupling of the band-edge multiplet of states to the broadband plasmonic resonance. Due to the resulting fast rate of energy exchange the strong coupling regime is reached and besides the exciton also the otherwise quenched trion state couples strongly with the slit resonator resulting in a four-peaked spectrum under strong-coupling conditions.

Invited Talk TT 57.3 Thu 10:30 HSZ 02

High efficiency and directional emission from a nanoscale light source in a planar optical antenna — •Mario Agio — Laboratory of Nano-Optics, University of Siegen, 57072 Siegen, Germany

Light emission and absorption are critical to applications such as lighting, sensing and information technology. Despite fundamental progress in the manipulation of light-matter interaction, coupling electromagnetic modes to nanoscale sources and detectors with a very high efficiency remains a challenge. Here, we introduce a simple planar antenna structure based on thin-film optics that attains more than 90% outcoupling efficiency and, at the same time, directional emission with a semiangle below 10 degrees [1,2]. Our findings are particularly relevant for materials with a high refractive index, like semiconductor-based nanophotonic devices, which typically exhibit a large mismatch to free-space and guided modes. Furthermore, our approach is general and thus applicable to any wavelength, provided that materials with the required optical properties are available. Finally, we discuss some results in the context of solid-state singlephoton sources.

[1] S. Checcucci et al., Light: Science & Applications 6, e16245 (2017). [2] H. Galal, M. Agio, to be submitted.

Coffee Break

Invited Talk TT 57.4 Thu 11:30 HSZ 02
Tailoring quantum states by measurement — •Jörg Wrachtrup — Institute for Quantum Science and Technology, IQST, University of Stuttgart, 70569 Stuttgart, Germany

Measurement induced back action is a unique property of quantum mechanics. It is a central challenge for a variety of applications, like error correction. However, it is also a unique tool in e.g. dissipative generation of entanglement or ground state cooling. In my talk, I will describe ways to control spin quantum states by tailored photonic measurements. I will describe of how to extend those measurement to a general scheme also, e.g. allowing to cool mesoscopic elements like mechanical oscillators.

Invited Talk TT 57.5 Thu 12:00 HSZ 02
Quantum optics and quantum control at the nanoscale with surface plasmon polaritons — •Stéphane Guérin — UMR 6303 CNRS-Université Bourgogne Franche-Comté, 21078 Dijon, France

The quantum control of emitters is a key issue for quantum information processing at the nanoscale. This generally necessitates the strong coupling of emitters to a high Q-cavity for efficient manipulation of the atoms and field dynamics (cavity quantum electrodynamics or cQED). Since almost a decade, strong efforts are put to transpose cQED concepts to plasmonics in order to profit of the strong mode confinement of surface plasmons polaritons [1]. Despite the intrinsic presence of lossy channels leading to strong decoherence in plasmonics systems, it has been experimentally proven that it is possible to reach the strong coupling regim [2]. In this work, we derive an effective Hamiltonian [3,4], which allows us to describe the metallic nanoparticle-emitter interaction in full analogy with cQED formalism using a multimodal lossy cavity. We discuss (i) the concept of dressed states of quantum emitter strongly coupled to a metal nanoparticle [5], leading for instance to efficient/blockade population transfers or superradiance/subradiance effects, and (ii) the multi-emitter adiabatic control via quantum plasmonics, for instance via stimulated Raman adiabatic processes [3].

[1] M.S. Tame, et al., Nature Physics 9, 329 (2013). [2] G. Zengin, et al., Phys. Rev. Lett. 114, 157401 (2015). [3] B. Rousseaux, et al., Phys. Rev. B 93, 045422 (2016). [4] D. Dzsotjan, et al., Phys. Rev. A 94, 023818 (2016). [5] H. Varguet, et al., Opt. Lett. 41, 4480 (2016).

TT 58: Focus Session on 2D Materials: Ballistic Quantum Transport in Graphene (jointly with DY, DS, HL, MA, O)

Ballistic electron waves yielded a plethora of insights already in 2D semiconducting heterostructures. Recent experimental techniques have paved the way to this regime also for graphene. The massless, relativistic, and chiral nature of its charge carriers enriches ballistic transport by qualitatively new physical phenomena, such as ambipolar states near pn-junctions, Klein tunneling, or a zeroth Landau level in a perpendicular magnetic field. This session will review the actual status.

Organisation: Wolfgang Häusler, Universität Augsburg; Reinhold Egger, Universität Düsseldorf; Klaus Richter, Universität Regensburg

Time: Thursday 9:30–13:00 Location: HSZ 03

Invited Talk TT 58.1 Thu 9:30 HSZ 03
Kondo Screening of a Vacancy Magnetic Moment in Graphene — •Eva Y. Andrei — Dept. of Physics, Rutgers University, Piscataway, NJ

Graphene in its pristine form has transformed our understanding of 2D electron systems leading to fundamental discoveries and to the promise of important applications. When the perfect honeycomb lattice of graphene is disrupted by single atom vacancies new phenomena emerge including the buildup of local charge and the appearance of a local moment. Using scanning tunneling microscopy to identify Kondo screening of the vacancy moment by its spectroscopic signature, we demonstrate that the local magnetic moment can be controlled either by doping or through the local curvature. This allows to detect and map the quantum phase transition separating magnetic from nonmagnetic states in this pseudogap system.

Invited Talk TT 58.2 Thu 10:00 HSZ 03
Higher-Than-Ballistic Conduction in Viscous Electron Fluids — •Leonid Levitov — Physics Department, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge MA02139

This talk will argue that in viscous electron flows interactions facilitate transport, allowing conductance to exceed the fundamental Sharvin-Landauer quantum-ballistic limit. The effect is particularly striking for the flow through a viscous point contact, a constriction exhibiting the quantum-mechanical ballistic transport at zero temperature but governed by electron hydrodynamics at elevated temperatures. The crossover between the ballistic and viscous regimes occurs when the mean free path for e-e collisions becomes comparable to the constriction width. Further, we will discuss the negative nonlocal response, a signature effect of viscous transport. This response exhibits an interesting nonmonotonic behavior vs. temperature at the viscous-to-ballistic transition. The response is negative but small in the highly viscous regime at elevated temperatures. The value grows as the temperature is lowered and the system becomes less viscous, reaching the most negative values in the crossover region where the mean free path is comparable to the distance between contacts. Subsequently, it reverses sign at even lower temperatures, becoming positive as the system enters the ballistic regime. This peculiar behavior provides a clear signature of the ballistic-to-viscous transition and enables a direct measurement of the electron-electron collision mean free path.

Invited Talk TT 58.3 Thu 10:30 HSZ 03
Electron Optics in Ballistic Graphene — •Ming-Hao Liu — Department of Physics, National Cheng Kung University

Electrons in clean graphene are known to behave like "charged photons" due to its celebrated energy dispersion linear in momentum, providing an ideal platform for exploring electron optics. Despite the discovery of graphene in 2004, devices of ultraclean samples with micron-scale mean free paths became accessible only recently. Reliable quantum transport simulations in the ballistic limit for understanding and predicting high-quality transport experiments have therefore become increasingly demanded nowadays. In this talk, an overview of our recent progress on simulating a variety of ballistic graphene transport experiments will be given, such as Fabry-Pérot interference, snake states, and gate-defined electron waveguides [1]. Keys to such quantum transport simulations will be briefly introduced [2]. Ongoing works possibly including *pnp* junctions in the presence of 2D Moiré superlattice and Weiss oscillation due to 1D periodic gating will be mentioned at the end of the talk.

[1] P. Rickhaus *et al.*, Nat. Communs. **4**, 2342 (2013); M. Drienovsky *et al.*, Phys. Rev. B **89**, 115421 (2014); A. Varlet *et al.*, Phys. Rev. Lett. **113**, 116601 (2014); P. Rickhaus *et al.*, Nat. Communs. **6**, 6470 (2015); P. Rickhaus *et al.*, Nano Lett. **15**, 5819 (2015).
[2] M.-H. Liu *et al.*, Phys. Rev. Lett. **114**, 036601 (2015).

15 min. break.

Invited Talk TT 58.4 Thu 11:15 HSZ 03
Ballistic Transport in Mesoscopic Graphene Devices — •Christoph Stampfer — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

The recent technological advances in encapsulating graphene by hexagonal boron nitride forming artificial van-der-Waals heterostructures allows the fabrication of graphene devices with high electronic quality. Outstanding charge carrier mobilities and mean free paths with more

than 10 micrometer are now accessible making this material stack interesting for studying ballistic transport. By further structuring the graphene-hBN based heterostructures mesoscopic devices can be fabricated on which phase coherent ballistic quantum transport can be studied.

Here, I will present low-temperature magneto-transport measurements on both (i) graphene quantum point contacts and (ii) high mobility graphene rings encapsulated in hexagonal boron nitride. Our experiments allow to extract information on quantized conductance, renormalized Fermi velocities close to the charge neutrality point as well as the co-existence of weak localization, Aharonov-Bohm oscillations and universal conductance fluctuations in graphene rings.

Invited Talk TT 58.5 Thu 11:45 HSZ 03

Interaction-Induced Conductance from Zero Modes in a Magnetic Graphene Waveguide — •Alex Zazunov — Heinrich-Heine-Universität Düsseldorf

We consider a waveguide formed in a clean graphene monolayer by a spatially inhomogeneous magnetic field. The single-particle dispersion relation for this waveguide exhibits a zero-energy Landau-like flat band, while finite-energy bands have dispersion and correspond, in particular, to snake orbits. For zero-mode states, all matrix elements of the current operator vanish, and a finite conductance can only be caused by virtual transitions to finite-energy bands. We show that Coulomb interactions generate such processes. In stark contrast to finite-energy bands, the conductance is not quantized and shows a characteristic dependence on the zero-mode filling. Transport experiments thereby offer a novel and highly sensitive probe of electron-electron interactions in clean graphene samples.

TT 58.6 Thu 12:15 HSZ 03

Ballistic thermophoresis on graphene — •Emanuele Panizon[1], Roberto Guerra[1,2], and Erio Tosatti[1,2,3] — [1]SISSA, Trieste, Italy — [2]CNR-IOM Democritos, Trieste, Italy — [3]ICTP, Trieste, Italy

The textbook thermophoretic force acting on a diffusing body in a fluid is proportional to the local temperature gradient. This is not the case for a diffusing physisorbed body on a submicron sized 2D suspended layer. A Non-Equilibrium Molecular Dynamics study of a test nanosystem - a gold nanocluster adsorbed on a single graphene sheet of length L clamped between two temperatures ΔT apart - reveals a phoretic force that is parallel to, but essentially independent of, the gradient magnitude $\Delta T/L$ up to a substantial L of $150nm$.

This is argued to represent ballistic thermophoresis, where the force is provided by the flux of massively excited flexural phonons, whose flow is in turn known to be ballistic and distance-independent up to relatively long scattering lengths before the eventual onset of the more standard diffusive regime. The surprising thrust and real momentum provided by the flexural modes are analysed and understood in terms of the large mass non/uniformity involved with these modes. The ensuing surf-riding of adsorbates on the vibrating 2D hard sheet, and the resulting gradient independent thermophoretic force, are not unlikely to possess practical applications.

TT 58.7 Thu 12:30 HSZ 03

Quantum time mirrors in two-band systems with and without broken time-reversal symmetry — •Phillipp Reck[1], Cosimo Gorini[1], Arseni Goussev[2], Viktor Krueckl[1], Mathias Fink[3], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Department of Mathematics, Physics and Electrical Engineering, Northumbria University, Newcastle Upon Tyne, UK — [3]Institut Langevin, ESPCI, CNRS, PSL Research University, Paris

Both metaphysical and practical considerations intrigued generations of scientists to devise and implement time-inversion protocols – in particular the Hahn echo [1], different forms of "time mirrors" for classical waves (see e.g. [2]), and recently an instantaneous time mirror for water waves [3]. With our proposal for an instantaneous Quantum Time Mirror [4], we showed the possibility to extend the family of time reversal protocols to *continuous quantum* systems, more precisely to wave packets in Dirac-cone systems, by changing the propagation direction with a short, time-dependent pulse.

In this talk, we discuss the effect on the Quantum Time Mirror of both, a static, out-of-plane magnetic field, which breaks time-reversal symmetry, and band structures other than the Dirac cone, e.g. the valence and conduction bands in direct gap semi-conductors.

[1] E. L. Hahn, Spin echoes. Phys. Rev.. 80, 580 (1950)

[2]M. Fink, IEEE Trans. Ultrason. Ferroelectr. Freq. Control, 39, 555, (1992)

[3]V. Bacot, et al., Nat. Phys. 12, 972–977 (2016)

[4]P. Reck, et al., arXiv:1603.07503 (2016)

TT 58.8 Thu 12:45 HSZ 03

Current flow paths in deformed graphene and carbon nanotubes — Erik Kleinherbers, •Nikodem Szpak, and Ralf Schützhold — Faculty of Physics, University of Duisburg-Essen, Germany

Due to imminent applications in nanoelectronics it is of high interest to understand the precise conductance properties of deformed graphene and bent carbon nanotubes. Since low-energy electronic excitations behave like massless Dirac fermions the current flow can be approximated semiclassically and used as a guide in the design of conducting nanoelectronic elements and nanosenors. Taking into account the curvature effects as well as an emerging inhomogeneous pseudo-magnetic field we calculate the current flow paths theoretically and compare them with numerical simulations of the full electronic transport.

TT 59: Superconductivity: Fe-based Superconductors - FeSe and others

Time: Thursday 9:30–12:15 Location: HSZ 103

TT 59.1 Thu 9:30 HSZ 103

Phonon spectrum of single-crystalline FeSe — •Tobias Engelhardt[1], Khalil Zakeri Lori[1], Thomas Wolf[2], and Matthieu Le Tacon[2] — [1]Heisenberg Spin-dynamics Group, Physikalisches Institut, Karlsruhe Institute of Technology, Wolfgang-Gaede-Str. 1, D-76131 Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruhe Institute of Technology, Hermann-v.-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany

Iron selenide is structurally the simplest iron-based superconductor and has been investigated extensively during the past years. Several experimental tools have been used to investigate the collective excitations, e.g. phonons, in this material. However, due to the lack of large single crystals, most of those experiments are performed on polycrystalline or powder samples. We report on the first phonon spectrum probed on the FeSe(001) surface by means of high-resolution electron energy-loss spectroscopy. Single crystals of FeSe are cleaved under ultra-high vacuum conditions and are subsequently measured above and below the nematic transition temperature. We observe five phonon modes and a phonon cutoff energy of about 42 meV at the center of Brillouin zone. These phonon modes disperse rather weakly while changing the momentum from zero up to the zone boundary, indicating that they are mainly of optical nature. We identify the origin of each phonon mode by comparing the experimental results to the ones of *ab initio* density functional calculations. Finally we comment on the role of temperature on the phonon spectrum.

TT 59.2 Thu 9:45 HSZ 103

Temperature evolution of the band structure of FeSe — •Yevhen Kushnirenko[1], Alexander Fedorov[1,2], Erik Haubold[1], Timur Kim[3], Moritz Hoesch[3], Thomas Wolf[4], Bernd Büchner[1], and Sergey Borisenko[1] — [1]IFW-Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Physikalisches Institut, Universit at zu Köln, Zulpicher Strasse 77, 50937 Köln, Germany — [3]Diamond Light Source, Harwell Campus, Didcot, OX11 0DE, United Kingdom — [4]Institut für Festkörperphysik, Karlsruhe Institute for Technology, Karlsruhe 76021, Germany

We have studied an evolution of the band structure of FeSe in a wide temperature range using angle-resolved photoemission spectroscopy (ARPES). We investigated the behavior of the hole-like bands in the center of the Brillouin zone and electron-like bands in its corners. We have shown that all these dispersions move with temperature as a function of binding energy. Remarkably, a direction of these shifts is different for the center and the corners of the Brillouin zone. This band structure behavior is observed for the orthorhombic state of FeSe (T<86K) as well as for the tetragonal state (T>86K).

TT 59.3 Thu 10:00 HSZ 103

Nodeless superconductivity and impurity bound states in FeSe single crystals — •Sahana Roessler[1], Lin Jiao[1], Chien-Lung Huang[1], Cevriye Koz[1], Ulrich K. Roessler[2], Ulrich Schwarz[1], and Steffen Wirth[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]IFW-Dresden, Institute for Solid State Research, D-01171 Dresden, Germany

We present the superconducting gap structure of FeSe single crystals [1,2] investigated by heat capacity and scanning tunneling microscopy/spectroscopy (STM/S). We show evidence for the existence of two superconducting gaps without nodes [3]. Further, the local density of states in the vicinity of a native selenium dumbbell in the superconducting state displays two resonant states inside the superconducting gap, equally spaced with respect to zero energy, but asymmetric in amplitude. The magnitude of the superconducting gap is found to be insensitive to the impurity potential, which confirms its non-magnetic nature. The in-gap bound states emerging from a non-magnetic impurity-induced pair-breaking suggest a sign changing pairing state in this material.

[1] C. Koz et al., Z. Anorg. Allg. Chem. 640, 1600 (2014)
[2] S. Rößler et al., PRB(R) 92, 060505 (2015)
[3] L. Jiao et al., arXiv:1605.01908 (2016)

TT 59.4 Thu 10:15 HSZ 103

Short-range quasi-static correlations in FeSe single crystals probed by μSR — •Vadim Grinenko[1], Rajib Sarkar[1], Philipp Materne[1], Sirko Kamusella[1], Hubertus Luetkens[2], Jean-Christophe Orain[2], Tatsuo Goko[2], Robert Scheuermann[2], Aichi Yamashita[3], Yoshihiko Takano[3], Yue Sun[4], Tsuyoshi Tamegai[4], Dmitriy Efremov[5], Stefan-Ludwig Drechsler[5], and Hans-Henning Klauss[1] — [1]Institute for Solid State Physics, TU Dresden, D-01069, Germany — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute (PSI), CH-5232 Villigen, Switzerland — [3]National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, 305-0047 JAPAN, Japan — [4]Department of Applied Physics, The University of Tokyo, Hongo, Tokyo 113-8656, Japan — [5]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

The FeSe system is an exception among the Fe based superconductors since it has a nematic transition at $T_s \sim 90$ K without long-range magnetic order down to lowest temperatures. The understanding of this phenomenon is a big challenge for a microscopic theory. We investigated high-quality single crystals of FeSe using zero field and high field muon spin rotation/relaxation (μSR) measurements. We observed that weak quasi-static local magnetic fields appear below 200 K in the entire sample volume. The static field inhomogeneity increases with the reduction of the temperature down to $T^* \sim 75$ K, where the transition to another magnetic state is observed. The evidence for the short-range quasi-static magnetic correlations well above T_s in FeSe provides a strong constraint for future microscopic theories.

TT 59.5 Thu 10:30 HSZ 103

Spatial variation of the two-fold anisotropic superconducting gap in a monolayer of $FeSe_{0.5}Te_{0.5}$ on a topological insulator — •Anand Kamlapure[1], Sujit Manna[1], Lasse Cornils[1], Torben Hänke[1], Martin Bremholm[2], Philip Hofmann[3], Jens Wiebe[1], and Roland Wiesendanger[1] — [1]Department of Physics, University of Hamburg, Hamburg, Germany — [2]Department of Chemistry and Center for Materials Crystallography, Aarhus University, Denmark — [3]Department of Physics and Astronomy, and Interdisciplinary Nanoscience Center iNANO, Aarhus University, Denmark

We present a low temperature scanning tunneling spectroscopy (STS) study of the superconducting properties of monolayers of $FeSe_{0.5}Te_{0.5}$ grown on the 3D topological insulator $Bi_2Se_{1.2}Te_{1.8}$. While the morphology and the overall transition temperature resemble those of similarly doped bulk crystals, the spectroscopic data shows a much larger spatial inhomogeneity in the superconducting energy gaps. Despite the gap inhomogeneity all the spectra can be described with a two-fold anisotropic s-wave gap function. The two-fold nature of the gap symmetry is evident from the Bogoliubov quasiparticle interference (QPI) pattern which shows distinct C_2 symmetric scattering intensities. We argue that the gap inhomogeneity emerges as a result of intrinsic disorder in our system similar to disordered conventional superconductors. Our system thus provides an ideal platform to study unconventional superconductivity in Fe chalcogenides in a single layer and in close proximity to a topological insulator.

TT 59.6 Thu 10:45 HSZ 103

Ultrathin FeSe films on Bi_2Se_3(0001) studied by STM and STS — •Jonas Warmuth, Udai Raj Singh, Verena Markmann, Jens Wiebe, and Roland Wiesendanger — Dept. of Physics, Hamburg University, Hamburg, Germany

Thin film iron chalcogenide superconductors have recently attracted interest due to an increase in transition temperatures as compared to the bulk material [1]. We report on the structural and electronic properties of ultrathin FeSe films grown on Bi_2Se_3(0001) [2]. Scanning tunnelling microscopy (STM) reveals FeSe thin films in the tetragonal phase with heights of one and two unit cells (UC) in respect to the Bi_2Se_3 surface. We observe striped moiré patterns and dumb-bell shaped defects on the FeSe films. Scanning tunnelling spectroscopy (STS) does not show any signature of a superconducting gap in the tunnelling spectra on the one and two UC thick FeSe islands down to 6.5 K [3]. These spectra rather show an asymmetric behaviour and a finite density of states at the Fermi level similar to spectra on bulk FeSe.

[1] I. Bozovic *et al* **2014** *Nature Physics* 10 892
[2] Y. Wang *et al* **2012** *J. Phys: Condensed Matter* 24 47
[3] U. Singh *et al* **2016** *J. Phys: Condensed Matter* 29 2

15 min. break.

TT 59.7 Thu 11:15 HSZ 103

Resonant scattering in the quasiparticle interference in superconducting LiFeAs — •Steffen Sykora[1], Zhixiang Sun[1], Pranab Kumar Nag[1], Jose Maria Guevara Parra[1], Danny Baumann[1], Rhea Kappenberger[1], Robert Beck[1], Sabine Wurmehl[1,2], Sergey Borisenko[1], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]IFW Dresden — [2]Institute for Solid State Physics, TU Dresden — [3]Center for Transport and Devices, TU Dresden

Probing the quasiparticle interference (QPI) by scanning tunneling microscopy/spectroscopy (STM) is an important tool to investigate the character of the superconducting state. We develop a theoretical model for the QPI in LiFeAs and compare the results with recent STM measurements of the Fourier transformed local density of states. Our selfconsistent t-matrix calculation goes beyond the standard Born approximation and is based on realistic band structure data. We find dominant QPI intensity at small transfer momentum in excellent agreement with the experiment. An unusual measured in-gap intensity is explained within the same theoretical framework by higher-order Andreev-scattering processes. The theoretical analysis reveals an important role of specific multiple scattering processes that lead to a resonant scattering mode at the energy scale of the superconducting gap. We discuss our results in the context of the pairing mechanism in LiFeAs.

TT 59.8 Thu 11:30 HSZ 103

Tunneling spectroscopy and long wavelength quasiparticle interference in LiFeAs — •Z. Sun[1], P. K. Nag[1], S. Sykora[1], S. Borensiko[1], D. Baumman[1], R. Kappenburger[1], R. Beck[1], S. Wurmehl[1], B. Büchner[1,2,3], and C. Hess[1,3] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden

We want present large-scale scanning tunneling spectroscopic map results on LiFeAs, especially focusing on the small momentum quasiparticle scatterings, where not much attention have been paid to previously. At the superconducting state, two particle-hole symmetric features are observed in the quasiparticle interference pattern: i) a large gap with a size of about 10 meV at 6.7 K; ii) ingap scatterings with small momentum transfer q close to zero. The evolution of the large gap size with temperature shows a mean field order parameter-like behavior with a critical temperature at T_c. For the large gap, we think that it reflects multiple scattering effects. And for the ingap particle-hole symmetric scatterings, we argue that they are due to the local variation of the superconducting order parameter caused by the defects and are related to Andreev reflection.

TT 59.9 Thu 11:45 HSZ 103

The quest for LaFeAsO single crystals — •Rhea Kappenberger[1,2], Saicharan Aswartham[1], Sebastian Selter[1], Francesco Scavaraggi[1,2], Federico Caglieris[1], A. U. B. Wolter[1], Christian Hess[1,3], Hans-Joachim Grafe[1], Sabine

Wurmehl[1,2], and Bernd Büchner[1,2,3] — [1]Leibniz Institute for Solid State and Materials Research Dresden IFW, Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, 01069 Dresden, Germany — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

Since the discovery of Fe-based superconductors in 2008, a lot of progress in crystal growth has been made in the 11, 111 and 122 systems. However, in the 1111 systems large crystals of high quality are very difficult to obtain, which renders investigations which crucially rely on single crystals, e.g. investigations of nematicity, practically impossible.

In this work, we present a novel approach of obtaining large La(Fe,Co)AsO and LaFeAs(O,F) single crystals using solid state synthesis and flux growth under ambient pressure. We were able to map out a new electronic phase diagram using single crystals of La(Fe,Co)AsO by several techniques such as structural, magnetic and resistivity measurements.

TT 59.10 Thu 12:00 HSZ 103

Lattice-assisted nematic order in $Ca_{10}Pt_3As_8(Fe_{1-x}Pt_xAs)_{10}$ — •Felix Brückner, Vadim Grinenko, Rajib Sarkar, Maksym Surmach, Dmytro Inosov, and Hans-Henning Klauss — Institut für Festkörperphysik, Technische Universität Dresden, Dresden, Germany

A broken 4-fold rotational symmetry, caused by electronic correlation effects, known as nematicity, is a well established fact in many iron-based superconductors. Slanted stacking of crystallographic layers can influence the formation of nematic order. This is investigated at the example of the triclinic system $Ca_{10}Pt_3As_8(Fe_{1-x}Pt_xAs)_{10}$. We present a joint study including magnetostriction, anisotropic resistivity, NMR and inelastic neutron scattering.

A phase transition at $T^* \approx 40$ K, far above the superconducting $T_c = 13$ K, manifests itself in a change in magnetic dynamic properties and a weak nematic lattice transition as well. NMR studies show a drastic decrease of low-energy magnetic fluctuations and a slight static broadening, interpreted as the opening of a pseudo spin-gap. A peak in the INS spectrum at the antiferromagnetic peak is found below the transition temperature. Since the nematic transition is twinned, we can observe the inequivalence of (1,1,0) and (1,-1,0) directions by applying magnetic field that detwins the sample and by measuring magnetostriction and resistivity. Beside the phase transition at T^* we found a second magnetic phase transition at ≈ 4 K.

TT 60: Correlated Electrons: f-Electron Systems

Time: Thursday 9:30–13:15 Location: HSZ 201

TT 60.1 Thu 9:30 HSZ 201

Fermi-surface evolution in the $Nd_xCe_{1-x}CoIn_5$ doping series — •J. Klotz[1,2], E. Green[1], K. Götze[1], C. Petrovic[3], I. Sheikhin[4], J.-H. Park[5], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Brookhaven National Laboratory, Brookhaven, USA — [4]Laboratoire National des Champs Magnétiques Intenses, Grenoble, France — [5]National High Magnetic Field Laboratory, Tallahassee, USA

$CeCoIn_5$ is one of the prime examples for heavy-fermion (HF) superconductivity [1]. However, superconductivity vanishes upon Nd doping on the Ce site [2]. Since there are several theory studies suggesting a relation of the Fermi-surface (FS) geometry and superconductivity, e. g. [3], the knowledge of the Fermi surface is of vital importance. Here, we present quantum-oscillation data of $Nd_xCe_{1-x}CoIn_5$ obtained using a rotatable torque magnetometer in fields up to 35 T and temperatures down to 50 mK. In combination with band-structure calculations, our data reveal only a subtle change in the cylindrical FS sheet of $CeCoIn_5$, but a strong change in the effective-mass renormalization.

[1] C. Petrovic, P. G. Pagliuso *et al.* J. Phys.: Condens. Matter **13**, L337 (2001).
[2] R. Hu, Y. Lee *et al.* Phys. Rev. B **77**, 165129 (2008).
[3] T. Moriya, Y. Takahashi, and K. Ueda, J. Phys. Soc. Jpn. **59**, 2905 (1990).

TT 60.2 Thu 9:45 HSZ 201

Investigation of the energy scales in SmB_6 by scanning tunneling microscopy — •Lin Jiao[1], Sahana Rössler[1], Dae-Jeong Kim[2], Liu Hao Tjeng[1], Zachary Fisk[2], Frank Steglich[1], and Steffen Wirth[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Physics, University of California, Irvine, California, USA

SmB_6 has been proposed as a topological Kondo insulator, which possesses topologically protected nontrivial surface states inside the bulk hybridization gap. By conducting scanning tunneling microscopy and spectroscopy, we are able to perform local measurements on well identified non-reconstructed (001) surfaces. Above ∼7 K and up to 80 K, the electronic states in SmB_6 are governed by the Kondo effect of the bulk [1]. At temperatures as low as 0.35 K, we observed several well-resolved states within the hybridization gap (±20 meV) of SmB_6 for the first time [2]. These states possess sharp peak-like features with a strong temperature dependence below 7 K, which indicates an additional energy scale at the surface of SmB_6, in line with a suppression of the Kondo effect at the surface. These high resolution data offer the opportunity to directly compare our spectroscopy with band structure calculations, and analyze their surface or bulk origin, which may help reconciling many contradicting assertions in this material.

[1] S. Rößler *et al.*, Proc. Natl. Acad. Sci. USA 111, 4798 (2014)
[2] L. Jiao *et al.*, Nat. Commun. 7, 13762 (2016)

TT 60.3 Thu 10:00 HSZ 201

Subsurface electronic structure of the mixed-valent SmB_6 — •Chul-Hee Min[1], Peter Lutz[1], Katharina Treiber[1], Thiago R.F. Peixoto[1], Hendrik Bentmann[1], Boyoun Kang[2], Beongki Cho[2], and Friedrich Reinert[1] — [1]Universität Würzburg, EP7, Würzburg, Germany — [2]School of Materials Science and Engineering, Gwangju Institute of Science and Technology (GIST), Gwangju, Korea

Strongly correlated topological insulators are expected to show drastically distinct phenomena near the surface region [1,2] because the hybridization strength V_{cf} of bulk and surface can be different [3]. We present an investigation on the probing depth dependence of $4f$ states and $3d$ core-levels in samarium hexaboride (SmB_6) to identify the unique subsurface electronic properties. From both angle- and photon energy-dependent studies, we estimate the thickness of the subsurface layer, which shows different Sm valence from the bulk one. Based on our estimation, we discuss about the surface, subsurface and bulk contributions in the $4f$ spectra. Our results indicate that at least two-component are present in the soft x-ray $4f$ spectra, which brings the size of the bulk gap of SmB_6 into question.

[1] Y. Xu, et al., Phys. Rev. Lett. 116, 246403 (2016).
[2] O. Erten, et al. Phys. Rev. Lett. 116, 046403 (2016).
[3] J. Allen, Phil. Mag. 96, 3227 (2016).

TT 60.4 Thu 10:15 HSZ 201

Excitons in topological Kondo insulators - theory of thermodynamic and transport anomalies in SmB_6 — •Johannes Knolle and Nigel R. Cooper — TCM Cavendish Laboratory, Univer- sity of Cambridge, UK

Kondo insulating materials lie outside the usual dichotomy of weakly versus correlated - band versus Mott - insulators. They are metallic at high temperatures but resemble band insulators at low temperatures because of the opening of an interaction induced band gap. The first discovered Kondo insulator (KI) SmB_6 has been predicted to form a topological KI (TKI) which mimics a topological insulator at low temperatures. However, since its discovery thermodynamic and transport anomalies have been observed that have defied a theoretical explanation. Enigmatic signatures of collective modes inside the charge gap are seen in specific heat, thermal transport and quantum oscillation experiments in strong magnetic fields. Here, we show that TKIs are susceptible to the formation of excitons and magneto-excitons. These charge neutral composite particles can account for long-standing anomalies in SmB_6 which is crucial for the identification of bulk topological signatures.

TT 60.5 Thu 10:30 HSZ 201

Magnetic field dependence of spin excitations in CeB_6 — P. Y. Portnichenko[1], S. V. Demishev[2], A. V. Semeno[2], H. Ohta[3], A. S. Cameron[1], M. A. Surmach[1], H. Jang[4,5], A. V. Dukhnenko[6], N. Yu. Shitsevalova[6], V. B. Filipov[6], A. Schneidewind[7], J. Ollivier[8], A. Podlesnyak[9], and •D. S. Inosov[1] — [1]TU Dresden, Germany — [2]General Physics Institute, Moscow — [3]Kobe University, Japan — [4]MPI für Festkörperphysik, Stuttgart — [5]National Accelerator Lab, Stanford, USA — [6]Inst. for Problems of Material Sciences, Kiev, Ukraine — [7]Forschungszentrum Jülich, Germany — [8]ILL, Grenoble, France — [9]SNS, Oak Ridge, USA

We employ inelastic neutron scattering (INS) to study the field dependence of spin fluctuations in CeB_6. The exciton shows no field splitting in marked contrast to $CeCoIn_5$. Instead, we observe a second field-induced magnon whose energy increases with field. At the ferromagnetic zone center, however, we find only a single mode with a nonmonotonic field dependence. At low fields, it is initially suppressed to zero together with the antiferromagnetic order parameter, but then reappears at higher fields inside the hidden-order phase, following the energy of an electron spin resonance (ESR). This is a unique example of a ferromagnetic resonance in a heavy-fermion metal seen by both ESR and INS consistently over a broad range of magnetic fields.

TT 60.6 Thu 10:45 HSZ 201

The quartet ground state in CeB_6: an inelastic x-ray scattering study — •Martin Sundermann[1,2], Kai Chen[1], Hasan Yavaş[3], Zachary Fisk[4], Maurits Haverkort[2,5], Liu Hao Tjeng[2], and Andrea Severing[1,2] — [1]University of Cologne, Institute of Physics II, 50937 Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]PETRA III, Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany — [4]Department of Physics and Astronomy, University of California, Irvine, CA 92697, USA — [5]*present address*: Institute for Theoretical Physics, Heidelberg University, 69120 Heidelberg, Germany

We investigated the ground state symmetry of the cubic hidden order compound CeB_6 by means of core level non-resonant inelastic x-ray scattering (NIXS). The information is obtained from the directional dependence of the scattering function that arises from higher than dipole transitions. Our new method confirms that the paramagnetic ground state is well described using a localized crystal-field model assuming a Γ_8 quartet ground state.

TT 60.7 Thu 11:00 HSZ 201

Hard axis ordering in ferromagnetic YbNiSn — •Dmitry Sokolov[1,2], Andrew Huxley[2], and Franz Demmel[3] — [1]MPI, CPfS, Dresden, Germany — [2]The University of Edinburgh, UK — [3]ISIS Facility, Rutherford Appleton Laboratory, Chilton, UK

We report on magnetic field induced critical points in ferromagnetic heavy fermion YbNiSn. We show via direct measurements of the static and dynamic magnetic susceptibility and also via bulk measurements that the ferromagnetism can be suppressed to zero temperature by a modest magnetic field of 1.7 T. Our neutron diffraction find a canted ferromagnetism in YbNiSn, in which the orientation of the ordered moment can be flipped by the magnetic field of 1 T. Above the field of 1 T the ordered moment attains a much higher value indicating a true easy axis. Our inelastic neutron scattering measurements find a gapped spin wave excitation, which softens at the field induced moment-reorientation transition at 1 T. As the magnetic field approaches 1.7 T transition into a fully polarized state the excitation loses its intensity and disappears. We discuss the origin of the hard-axis ordering and the soft mode in this material.

15 min. break.

TT 60.8 Thu 11:30 HSZ 201

Direct bulk sensitive probe of $5f$ symmetry in URu_2Si_2 — Martin Sundermann[1], Maurits W Haverkort[2,4], Mark Golden[3], Yinkai Huang[3], Anne de Visser[3], Peter Thalmeier[2], Liu Hao Tjeng[2], and •Andrea Severing[1] — [1]University of Cologne, Institute of Physics II, 50937 Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Van der Waals-Zeeman Institute, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands — [4]present address: Institute for Theoretical Physics, Heidelberg University, 69120 Heidelberg, Germany

The order parameter of the second-order phase transition into a hidden order phase in URu_2Si_2 is still a mystery, despite 30 years of research. However, it is understood that the symmetry of the order parameter must be related to the symmetry of the low lying local electronic f-states. Here we present results of a novel spectroscopy, namely core-level non-resonant inelastic x-ray scattering (NIXS). This method allows for the measurement of local high-multipole excitations and it is bulk sensitive. The observed anisotropy of the scattering function unambiguously shows that the $5f$ ground state wave function is composed mainly of the Γ_1 with majority $J_z = |4\rangle + |-4\rangle$ and/or Γ_2 singlet states. The incomplete dichroism indicates the superposition of quantum states necessary for constructing the HO state with the breaking of the fourfold symmetry.

TT 60.9 Thu 11:45 HSZ 201

Field induced Lifshitz transition in UPt_2Si_2: Fermi surface under extreme conditions — Dirk Schulze Grachtrup[1], •Nico Steinki[1], Stefan Süllow[1], Zübeyir Cakir[2], Gertrud Zwicknagl[2], Yuriy Krupko[3], Marcelo Jaime[4], and John A. Mydosh[5] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, D-38106 Braunschweig, Germany — [2]Institut für Mathematische Physik, TU Braunschweig, D-38106 Braunschweig, Germany — [3]Laboratoire National des Champs Magnétiques Intenses (LNCMI-EMFL), CNRS, UGA, 38042 Grenoble, France — [4]National High Magnetic Field Laboratory, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — [5]Kamerlingh Onnes Laboratory, Leiden University, 2300RA Leiden, The Netherlands

We have measured Hall effect, magnetotransport and magnetostriction on the field induced phases of single crystalline UPt_2Si_2 in magnetic fields up to 60 T at temperatures down to 50 mK. For the magnetic field applied along the c axis we observe strong changes in the Hall effect at the phase boundaries. From a comparison to band structure calculations utilizing the concept of a dual nature of the uranium $5f$ electrons, we find evidence for field induced topological changes of the Fermi surface due to at least one Lifshitz transition. Furthermore, we find a unique history dependence of the magnetotransport and magnetostriction data, indicating that the Lifshitz type transition is of a discontinuous nature, as predicted for interacting electron systems.

TT 60.10 Thu 12:00 HSZ 201

Microwave response of $CeCu_2Si_2$ — •Markus Thiemann[1], Martin Dressel[1], Silvia Seiro[2], Christoph Geibel[2], Nicholas Lee-Hone[3], David Broun[3,4], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [3]Department of Physics, Simon Fraser University, Burnaby, Canada — [4]Canadian Institute for Advanced Research, Toronto, Canada

$CeCu_2Si_2$ is a heavy fermion compound, exhibiting a onset of superconductivity ($T_c \approx 0.6$K) at a quantum critical point. Although superconductivity in this compound was discoverd over 30 years ago, its origin and the symmetry of the order parameter still remain unclear. While it was long believed that the order parameter had a d-symmetry, supported by neutron scattering experiments and NQR, recent specific heat measurements indicate fully gapped multigap superconductivity. Since the relevant energy scales of this compound are in the μeV regime, microwave measurements are an adequate technique to reveal intrinsic electronic properties of this system.

We performed microwave resonator measurements in a frequency and temperature range from 2.5GHz to 20GHz and 0.1K to 10K. This enabled us to determine the complex optical conductivity in the metallic as well as the superconducting state. In the metallic state, above 0.6K we see signs of the heavy fermion state arising, pushing the scattering rate towards our spectral range. In the superconducting state the absense of a coherence peak and the temperature dependence of the superfluid density point towards unconventional superconductivity.

TT 60.11 Thu 12:15 HSZ 201

Ising-type Magnetic Anisotropy in $CePd_2As_2$ — •M. O. Ajeesh[1], T. Shang[2], W. B. Jiang[2], W. Xie[2], R. D. dos Reis[1], M. Smidman[2], C. Geibel[1], H. Q. Yuan[2], and M. Nicklas[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Center for Correlated Matter and Department of Physics, Zhejiang University, Hangzhou, China

We studied the magnetic, thermal, and electrical transport properties of $CePd_2As_2$. X-ray diffraction confirmed the tetragonal $ThCr_2Si_2$-type structure and the high-quality of the single crystals. Magnetization and magnetic susceptibility data taken along the different crystallographic directions evidence a huge crystal electric field (CEF) in-

duced Ising-type magneto-crystalline anisotropy with a large c-axis moment and a small in-plane moment at low temperature. Accordingly, we observe a uniaxial antiferromagnetic (AFM) ordering at a transition temperature of $T_N \approx 15$K with the crystallographic c-direction being the magnetic easy axis. The magnetic entropy gain up to T_N reaches almost $R\ln 2$ indicating localized $4f$-electron magnetism without significant Kondo-type interactions. Below T_N, the application of a magnetic field along the c-axis induces a metamagnetic transition from the AFM to a field-polarized phase at $B_C \approx 1$T, exhibiting a text-book example of a spin-flip transition as anticipated for an Ising-type AFM. A detailed crystal electric field analysis based on the magnetic-susceptibility data indicates an almost pure $|\pm 5/2\rangle$ CEF ground-state doublet with the dominantly $|\pm 3/2\rangle$ and the $|\pm 1/2\rangle$ doublets at 290K and 330K, respectively.

TT 60.12 Thu 12:30 HSZ 201

Stress - Temperature Phase Diagram of Antiferromagnetic order in $CeAuSb_2$ Under Uniaxial Pressure — •Joonbum Park[1,2], Hideaki Sakai[3], Andrew P. Mackenzie[1,4], and Clifford W. Hicks[1] — [1]Max Planck Institute for Chemical Physics of Solids, Noethnitzer Strasse 40, 01187 Dresden, Germany — [2]Max Planck POSTECH Center for Complex Phase Materials, Max Planck POSTECH/Korea Research Initiative (MPK), Gyeongbuk 376-73, Korea — [3]Department of Physics, Osaka University, Toyonaka, Osaka 560-0043, Japan — [4]Scottish Universities Physics Alliance (SUPA), School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom

We present results of the electrical transport measurements under uniaxial pressure on the antiferromagnet $CeAuSb_2$. In the unstrained system, the resistivity along [100] shows a sharp drop at the Néel temperature ($T_N \approx 6.5$ K), suggesting a first order transition. With compression along [100] by ≈ 0.3 %, the transition splits into two continuous transitions, at temperatures T_1 and T_2. T_1 is fully suppressed at a compression of ≈ 0.6 %, and in pressure ramps at low temperature this transition is a sharp cusp with hysteresis, indicating a first-order transition. T_2, on the other hand, rises continuously with increasing compression, reaching 9 K at 1.2 % compression. At present, the nature of the strain-induced phase between T_1 and T_2 is not clear.

TT 60.13 Thu 12:45 HSZ 201

Incommensurate short-range multipolar order parameter of phase II in $Ce_3Pd_{20}Si_6$ — •Pavlo Y. Portnichenko[1], Silke Paschen[2], Andrey Prokofiev[2], Matthias Vojta[3], Alistair S. Cameron[1], Jean-Michel Mignot[4], Alexandre Ivanov[5], and Dmytro S. Inosov[1] — [1]IFP, TU Dresden, Germany — [2]Vienna Univ. of Technology, Austria — [3]ITP, TU Dresden, Germany — [4]LLB, France — [5]ILL, France

The clathrate compound $Ce_3Pd_{20}Si_6$ is a heavy-fermion metal that exhibits magnetically hidden order at low temperatures. Reputedly, this exotic type of magnetic ground state, known as "phase II", could be associated with the ordering of Ce $4f$ quadrupolar moments. In contrast to conventional (dipolar) order, it has vanishing Bragg intensity in zero magnetic field and, as a result, has escaped direct observation by neutron scattering until now. Here we report the observation of diffuse magnetic neutron scattering induced by an application of magnetic field along either the $[1\bar{1}0]$ or the [001] direction within phase II. The broad elastic magnetic signal that surrounds the (111) structural Bragg peak can be attributed to a short-range G-type antiferromagnetic arrangement of field-induced dipoles modulated by the underlying multipolar order on the simple-cubic sublattice of Ce ions occupying the 8c Wyckoff site. In addition, for magnetic fields applied along the [001] direction, the diffuse magnetic peaks in $Ce_3Pd_{20}Si_6$ become incommensurate, suggesting a more complex modulated structure of the underlying multipolar order that can be continuously tuned by a magnetic field.

TT 60.14 Thu 13:00 HSZ 201

Frustrated local moment magnetism in a metallic system: $Ce_6Ni_6P_{17}$ — •Diego Franco and Christoph Geibel — Max-Planck-Institut für Chemische Physik Fester Stoffe

Frustrated metallic systems are potentially of strong interest because the interaction between magnetic and itinerant degrees of freedom is expected to result in unusual properties. However the number of appropriate systems is extremely scarce. Because of its structure the polyphosphide $Ce_6Ni_6P_{17}$ is an attractive candidate. Ce atoms are located on the corners of octahedra, which form a body centered cubic lattice. Thus one might expect frustration within the octahedra and frustration because of the body centered arrangement of the octahedra [1]. A preliminary study provided some evidence for frustration, but presented only limited experimental results [1]. We synthesized polycrystalline samples and present magnetization, specific heat and resistivity data. Our results confirm $Ce_6Ni_6P_{17}$ to be a metallic, frustrated local moment system. Kondo interaction are negligible resulting in well-defined 4f local moments. Specific heat C(T)/T data evidence magnetic order at merely $T_N = 0.97$ K, with only a small anomaly at T_N compensated by a huge tail in C(T)/T extending far above T_N. The magnetic fluctuations indicated by this large tail in C(T)/T are also seen as a broad maximum in $\chi(T)$ at $T > T_N$. Thus $Ce_6Ni_6P_{17}$ is a very promising candidate for studying magnetic frustration in a metallic system.

[1] N. Takeda et al., J. Phys. : Conf. Series 391 (2012) 012071

TT 61: Correlated Electrons: (General) Theory 2

Time: Thursday 9:30–13:00 Location: HSZ 204

TT 61.1 Thu 9:30 HSZ 204

Magnetic response of spin-orbit coupled d-electrons in non-spherical potentials — •Daniil Toloui-Mantadakis, Marc Hoeppner, and Philipp Hansmann — Max Planck Institute for Solid State Research, Stuttgart, Germany

The Hubbard model and its multi-orbital extensions is one of the most prominent microscopic starting points to understand properties of ground state and low energy excitations. Its explicit formulation in terms of single particle operators and the effective Coulomb interaction crucially relies on approximations which are based on an assumed hierarchy of energy scales: while in 3d transition metal compounds crystal field effects dominate and yield good quantum numbers, in 4f rare-earth compounds (e.g. heavy fermion systems like CeX_2Si_2) strong spin-orbit coupling renders total angular momentum to be a much better single particle basis. However, a clear hierarchy is not always present and when we move towards the 4d and 5d compounds we can hardly define any good quantum numbers at all.

Here, we present a dynamical mean-field study of a generic three band model including both crystal field- and spin-orbit coupling operators on equal footing, using the fully SU(2) symmetric Coulomb interaction. We show the results of the two-particle uniform magnetic response which is, other than single particle spectra quantities, much more sensitive to effects of electronic correlations, and we compare them with the exact atomic limit ones.

TT 61.2 Thu 9:45 HSZ 204

Dual Fermion Approach for the Honeycomb Lattice — •Daniel Hirschmeier[1], Hartmut Hafermann[2], and Alexander I. Lichtenstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Germany — [2]Mathematical and Algorithmic Sciences Lab, France Research Center, Huawei Technologies Co. Ltd., Paris

The study of strongly correlated electron systems remains a hot topic in modern condensed matter physics due to its rich phenomenology and its wide range of applications. Lately the material graphene has become one of the most frequently studied objects in this field, having a number of interesting properties arising due to its extraordinary crystal structure.

In this work we explore the consequences of correlation effects for electrons on a lattice with the very same structure, by applying the recently developed Dual Fermion approach to the Hubbard model on the honeycomb lattice. The Dual Fermion approach is a multiscale diagrammatic expansion around the Dynamical Mean Field Theory incorporating non-local correlations.

We show that the Dual Fermion approach describes the occurence of non-trivial correlation effects like the formation of extended Van Hove singularities in the quasiparticle spectrum close to Van Hove filling. Furthermore we investigate the Hubbard model on the honeycomb lattice at half-filling. Our results show an exponential scaling of antiferromagnetic fluctuations with temperature, which is in

good agreement with analytical results and provide a revision of the semimetall-insulator scenario in DMFT.

TT 61.3 Thu 10:00 HSZ 204

Site-selective Mott insulator-metal transition and charge disproportionation in Fe_2O_3 under pressure — •Ivan Leonov — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — Materials Modeling and Development Laboratory, National University of Science and Technology 'MISIS', 119049 Moscow, Russia

We present a theoretical study of the electronic structure and phase stability of hematite (α-Fe_2O_3) near a pressure-induced Mott insulator-metal transition using the fully charge self-consistent DFT+DMFT approach. Our results reveal that upon compression above $\sim$ 45 GPa, Fe_2O_3 undergoes a Mott insulator (MI) to site-selective MI phase transition. The latter is characterized by a collapse of local magnetic moments and emergence of a metallic state only on half of the Fe sites. Our results suggest that the phase transition is accompanied a charge disproportionation of the Fe ions, implying a complex interplay between electronic correlations and the lattice. We explain the high-pressure behavior of Fe_2O_3 and suggest that it is primary a localized to itinerant moment behavior transition that gives rise to magnetic collapse of the Fe ions under pressure.

TT 61.4 Thu 10:15 HSZ 204

L-hole Pocket of the Palladium Fermi Surface Revealed by Positron Annihilation Spectroscopy — •Michael Sekania[1,2], Wilhelm Hans Appelt[3,4], Andreas Östlin[1], Liviu Chioncel[1,4], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Andronikashvili Institute of Physics, 0177 Tbilisi, Georgia — [3]Theoretical Physics II, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [4]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

The existence of the L-hole pocket of the palladium Fermi surface was extensively discussed in the past decades. Although scalar-relativistic density functional theory calculations are not able to reproduce this feature, it is expected that relativistic corrections, among them spin-orbit coupling, are strong enough to create an L-hole pocket. So far, no clear experimental evidence is reported in the literature. In our study we find that relativistic corrections indeed create such a L-hole pocket. Furthermore we show that the computed two dimensional Angular Correlation of Electron Positron Annihilation Radiation (the so called 2D-ACAR) clearly demonstrates the features associated with the L-hole pocket. We also show that electronic correlations do not alter these features significantly. A 2D-ACAR experiment should be able to resolve the disputes concerning the existence of the L-hole pocket in the Palladium Fermi surface.

TT 61.5 Thu 10:30 HSZ 204

Electronic Correlations in Vanadium Revealed by Electron-Positron Annihilation Measurements — Josef Andreas Weber[1], Diana Benea[2], Wilhelm Hans Appelt[3,4], Hubert Ceeh[1], Wolfgang Kreuzpaintner[1], Michael Leitner[1,5], Dieter Vollhardt[6], Christoph Hugenschmidt[1,5], and •Liviu Chioncel[4,6] — [1]Physik-Department, Technische Universität München, James-Franck Strasse, 85748 Garching, Germany — [2]Faculty of Physics, Babes-Bolyai University, Kogalniceanustr 1, 400084 Cluj-Napoca, Romania — [3]Theoretical Physics II, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [4]Augsburg Center for Innovative Technologies, University of Augsburg, 86135 Augsburg, Germany — [5]Heinz Maier-Leibnitz Zentrum, Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany — [6]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The electronic structure of vanadium measured by Angular Correlation of electron-positron Annihilation Radiation (ACAR) is compared with the predictions of the combined Density Functional and Dynamical Mean-Field Theory (DMFT). Reconstructing the momentum density from five 2D projections we were able to determine the full Fermi surface and found excellent agreement with the DMFT calculations. In particular, we show that the local, dynamic self-energy corrections contribute to the anisotropy of the momentum density and need to be included to explain the experimental results.

TT 61.6 Thu 10:45 HSZ 204

Influence of non-local interactions on the Mott metal-insulator transition. — •Malte Schüler[1,2], Erik G. C. P. van Loon[3], Mikhail I. Katsnelson[3], and Tim O. Wehling[1,2] — [1]Universtity of Bremen, Institute for Theoretical Physics — [2]Universtity of Bremen, Bremen Center for Computational Materials Science — [3]Radboud University, Institute for Molecules and Materials

We investigate how short- and long-ranged non-local Coulomb interactions influence the metal-insulator phase boundary of the half-filled Hubbard model on square lattices and honeycomb lattices. We find that generally, non-local interactions stabilize the Fermi-liquid regime and that the phase boundary behaves linearly with infinitesimal non-local interactions. We present an upper bound for the boundary's slope. Our findings help to elucidate if the Hubbard model can describe the Mott transition in real materials. For our investigations, we use a variational principle which maps extended Hubbard models to effective purely local Hubbard models. The mapping relies on Quantum Monte Carlo solutions of the the local Hubbard model.

15 min. break.

TT 61.7 Thu 11:15 HSZ 204

Lattice effects on the superfluid stiffness — •Matthias Hecker and Jörg Schmalian — TKM, KIT, Karlsruhe, Germany

The underdoped regime of the copper oxide superconductors with its rich set of physical features has been intensely debated over years, while the overdoped side, perceived as simple and said to follow a BCS behavior, has been mostly disregarded. In a recent experiment on the overdoped side of $La_{2-x}Sr_xCuO_4$ [1], yet, a stark contrast between the BCS prediction on the superfluid stiffness and the measurement outcome has been observed. We investigate whether the discrepancy in the superfluid stiffness can be rooted in the underlying lattice and the concomitant electronic dispersion relation. In particular, we work out the impact of fluctuation corrections to the superfluid stiffness in a Galilei-non-invariant system.

[1] Božović, I., He, X., Wu, J. & Bollinger, A.T., Nature **536**, 309 (2016).

TT 61.8 Thu 11:30 HSZ 204

The role of fluctuations for density-wave instabilities — •Mareike Hoyer[1,2], Sonja Fischer[3,1], and Jörg Schmalian[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Deutschland — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Deutschland — [3]Institute for Theoretical Physics, Universiteit Utrecht, Niederlande

Density-wave instabilities have been observed and studied in a multitude of materials. In particular, in the context of unconventional superconductors like the iron-based superconductors, they have excited considerable interest, since they compete with the superconducting state in these materials. We analyze the fluctuation corrections to the equation of state of the density-wave order parameter for commensurate charge and spin-density waves due to perfect nesting. For XY magnets, we find that contributions due to longitudinal and transverse fluctuations cancel each other, making the mean-field analysis of the problem controlled. This is consistent with the observation by Kos, Millis, and Larkin [1], who analyzed fluctuation corrections to the BCS theory of superconductivity. However, in case of charge-density waves and spin-density waves with Heisenberg symmetry, we find that fluctuation corrections are not negligible, and hence mean-field theories are not justified. These singular fluctuations originate from the intermediate length-scale regime, with wavelengths between the lattice constant and the $T = 0$ correlation length. We comment on strategies to resolve this challenge in the description of density-wave instabilities.

[1] Š. Kos, A. J. Millis, and A. I. Larkin, PRB **70**, 214531 (2004)

TT 61.9 Thu 11:45 HSZ 204

Numerical investigation of the reduction in the topological classification due to interactions in 2D — •Johannes S. Hofmann[1], Raquel Queiroz[2,3], Eslam Khalaf[2], and Fakher F. Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Würzburg, Deutschland — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Deutschland — [3]Weizmann Institute of Science, Rehovot, Israel

Symmetry protected topological phases have been classified for non-interacting models by A. P. Schnyder et. al.[1]. As first shown by Kitaev and Fidkowski[2] for class BDI in 1D and later extended to

all symmetry classes [3], interactions lead to a reduction of topologically distinct phases. R. Queiroz et. al. present explicit rules for the construction of such interactions [4].

Here we consider the symmetry class A' in 2 dimensions, i.e. models with time-reversal, particle-hole and a unitary $\mathbb{Z}_2$ symmetry R, where interactions reduce the topological classification from $\mathbb{Z}$ to $\mathbb{Z}_4$. We realize this class by a lattice Dirac Hamiltonian and the goal of this project is to first confirm the arguments provided in the previous studies numerically by explicitly connecting a topological phase with winding $n = 4$ adiabatically to the trivial insulator ($n = 0$). We then study the mechanism, how both the gap closing and the symmetry breaking, required in the non-interacting model, is avoided.

[1] Schnyder et. al., PRB 78, 195125
[2] Fidkowski and Kitaev, PRB 81, 134509
[3] Morimoto et. el., PRB 92, 125104
[4] Queiroz et. el., PRL 117, 206405

TT 61.10 Thu 12:00 HSZ 204

Gridless Stochastic Sampling: Analytic Continuation of Quantum Monte Carlo Data — •Khaldoon Ghanem and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

The stochastic sampling method (StochS) is used for the analytic continuation of quantum Monte Carlo data from the imaginary axis to the real axis. Although StochS does not have explicit parameters, the results depend on the discretization grid which acts as a default model.

To reduce the effect of the grid, we extend StochS into a gridless method (gStochS) by sampling the grid points from a default model instead of having them fixed. The effect of the default model is much reduced in gStochS compared to StochS and depends mainly on its width rather than its shape. The proper width can be then chosen using a simple recipe.

To avoid fixing the width, we go one step further and extend gStochS to sample over a class of default models with different widths. The method is then able to automatically relocate the grid points and concentrate them into the important region. Results show that gStochS gives good results and resolves sharp features in the spectrum without the need for fine tuning a default model.

TT 61.11 Thu 12:15 HSZ 204

Continuous-time quantum Monte Carlo for fermion-boson lattice models: Improved bosonic estimators and application to the Holstein model — •Manuel Weber, Fakher F. Assaad, and Martin Hohenadler — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We extend the continuous-time interaction-expansion quantum Monte Carlo method with respect to measuring observables for fermion-boson lattice models. Using generating functionals, we express expectation values involving boson operators, which are not directly accessible because simulations are done in terms of a purely fermionic action, as integrals over fermionic correlation functions. We also demonstrate that certain observables can be inferred directly from the vertex distribution, and present efficient estimators for the total energy and the phonon propagator of the Holstein model. Furthermore, we generalize the covariance estimator of the fidelity susceptibility to retarded interactions. The new estimators are applied to half-filled spinless and spinful Holstein models in one dimension. The observed renormalization of the phonon mode across the Peierls transition in the spinless model suggests a soft-mode transition in the adiabatic regime. The critical point is associated with a minimum in the phonon kinetic energy and a maximum in the fidelity susceptibility.

TT 61.12 Thu 12:30 HSZ 204

Relating correlation measures: the importance of the energy gap — •Carlos L. Benavides-Riveros[1], Nektarios Lathiotakis[2], Christian Schilling[3], and Miguel A. L. Marques[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle (Saale), Germany — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, GR-11635 Athens, Greece — [3]Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom

The concept of correlation is at the core of all approaches to describe many-body quantum systems. In general, multipartite correlation is a property that can be assigned to quantum states independent of the underlying physics (Hamiltonian). This is in contrast to quantum chemistry where the correlation energy (the energy not seized by the Hartree-Fock ansatz) plays a more prominent role. By concise means, we show that these two different viewpoints on the concept of correlation are closely related. By studying few site Hubbard models and the hydrogen dimer H_2 we relate popular fermionic correlation measures to the correlation energy and emphasize the role of the energy gap.

TT 61.13 Thu 12:45 HSZ 204

The Quantum-Statistical Condensate of One-Dimensional Anyons — •Thore Posske[1], Björn Trauzettel[2], and Michael Thorwart[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg — [2]Institut für Theoretische Physik und Astrophysik, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg

We develop an exact many-body formalism for one-dimensional anyons, the hybrid particles between bosons and fermions. Besides providing characteristic observables, we reveal the quantum-statistical condensate. This genuine many-body condensate is created purely by quantum-statistical attraction. It is potentially more stable than a Bose-Einstein condensate and carries a rich structure of degenerate internal excitations. Parallels to the Lieb-Liniger model of interacting bosons are discussed.

TT 62: Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 1

Time: Thursday 9:30–13:00 Location: HSZ 304

TT 62.1 Thu 9:30 HSZ 304

Proposal for measuring the finite-temperature Drude weight of integrable systems — Christoph Karrasch[1], Tomaz Prosen[2], and •Fabian Heidrich-Meisner[3] — [1]Dahlem Center for Complex Quantum Systems, FU Berlin, Germany — [2]Physics Department, University of Ljubljana, Slovenia — [3]Arnold Sommerfeld Center for Theoretical Physics, LMU Munich, Germany

Integrable models such as the spin-1/2 Heisenberg chain, the Lieb-Liniger or the one-dimensional Hubbard model are known to avoid thermalization, which was also demonstrated in several quantum-quench experiments. Another dramatic consequence of integrability is the zero-frequency anomaly in transport coefficients, which results in ballistic finite-temperature transport, despite the presence of strong interactions. While this aspect of nonergodic dynamics has been known for a long time, there has so far not been any unambiguous experimental realization thereof. We make a concrete proposal for the observation ballistic transport via local quantum quench experiments in fermionic quantum-gas microscopes. Such an experiment would also unveil the coexistence of ballistic and diffusive transport channels in one and the same system and provide a means of measuring finite-temperature Drude weights. The connection between local quenches and linear-response functions is established via time-dependent Einstein relations.

[1] Karrasch, Prosen, Heidrich-Meisner, arXiv:1611.04832

TT 62.2 Thu 9:45 HSZ 304

Dynamics of the transverse-field Ising model in 3D — •Markus Schmitt[1] and Markus Heyl[2] — [1]Institut für Theoretische Physik, Georg-August-Universität, Göttingen — [2]Max-Planck Institute for the Physics of Complex Systems, Dresden

We formulate the dynamics after a quench in the three-dimensional transverse-field Ising model in terms of classical partition sums, which can be evaluated using conventional Monte Carlo methods for classical spin systems with system sizes markedly beyond the capabilities of, e.g., exact diagonalization. In this way, we obtain insights into the time evolution of observables and dynamical quantum phase transitions in the Loschmidt echo, which we analyze in the vicinity of critical times similar to [M. Heyl, Phys. Rev. Lett. 115, 140602 (2015)].

TT 62.3 Thu 10:00 HSZ 304

An impurity solver for nonequilibrium dynamical mean field

theory based on hierarchical quantum master equations — •Rainer Härtle[1] and Andrew J. Millis[2] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]Department of Physics, Columbia University, New York, USA

We present a new impurity solver for real-time and nonequilibrium dynamical mean field theory applications, based on the recently developed hierarchical quantum master equation approach [1,2]. Our method combines a hybridization expansion of the time evolution operator, with an advanced, systematic truncation scheme [2]. Convergence to exact results for not too low temperatures has been demonstrated by a direct comparison to quantum Monte Carlo simulations [3]. The approach is time-local and does not require evolution from an uncorrelated initial condition, giving access to nonequilibrium steady states and to slow dynamics such as occur, e.g., in the presence of magnetic fields or exchange interactions [3–5]. Here, we present first results of this new scheme for the description of strongly correlated materials in the framework of dynamical mean field theory.

[1] Jin *et al.*, JCP 128, 234703 (2008)
[2] Härtle *et al.*, PRB 88, 235426 (2013)
[3] Härtle *et al.*, PRB 92, 085430 (2015)
[4] Härtle *et al.*, PRB 90, 245426 (2014)
[5] Wenderoth *et al.*, PRB 94, 121303R (2016)

TT 62.4 Thu 10:15 HSZ 304

Higgs-modes in non-equilibrium $d_{x^2-y^2}$-wave superconductors — •Andreas P. Schnyder[1], Holger Krull[2], Götz S. Uhrig[2], Nikolaj Bittner[1], and Dirk Manske[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart — [2]Technische Univerität Dortmund, 44221 Dortmund

The recently developed time-resolved ARPES technique has made it possible to measure collective modes in non-equilibrium quantum systems. Using an iterated equation of motion approach, we investigate the collective Higgs modes of non-equilibrium $d_{x^2-y^2}$-wave superconductors and simulate the corresponding time-resolved ARPES spectra. We find that in $d_{x^2-y^2}$-wave superconductors two different Higgs modes can be excited by the pump pulse. The relative strength of these two Higgs modes is controlled by the incident angle of the pump pulse. We determine the signatures of these Higgs modes in the time-resolved ARPES response.

TT 62.5 Thu 10:30 HSZ 304

Towards Mott-Insulator based Photovoltaic devices — •Max Sorantin[1], Antonius Dorda[1], Wolfgang von der Linden[1], Karsten Held[2], and Enrico Arrigoni[1] — [1]Institute for theoretical physics, TU Graz, Austria — [2]Institute for solid state physics, TU Vienna, Austria

Recently, Mott-insulating heterostructures have been proposed as candidates for highly efficient solar cells [1] owing to impact ionisation processes [2]. Previous works have investigated the doublon dynamics in such systems within time-dependent DMFT by looking at the time evolution after a photoexcitation [3]. In the present work we focus on the (quasi-) steady state of periodically driven correlated lattice systems within Floquet DMFT. We employ the Auxiliary Master Equation Approach (AMEA) [4] to solve the time averaged impurity problem and assess the validity of this approximation by comparison with Iterated Perturbation Theory (IPT) [5]. Our model consists of a correlated layer, subject to a periodic driving via a homogeneous electric field, coupled to leads with an applied bias voltage. Furthermore, we generalize the system to a multilayer structure where the additional layers are used to model an electric field gradient. Investigating the results for the double accupancy, current and Spectralfunction in dependence of the external driving frequency suggests that impact ionization plays a domniant role in the steady state dynamics.

[1] E. Assman et al., PRL 110 (2013)
[2] J. Coulter et al., PRB 90 (2014)
[3] M. Eckstein et al., PRL 113 (2014);
P. Werner et al., PRB 90 (2014)
[4] E. Arrigoni et al., PRL 110 (2013)
[5] A. Joura et al., PRB 91 (2015)

TT 62.6 Thu 10:45 HSZ 304

Thermoelectric response of the correlated layer - non-equilibrium DMFT study — •Irakli Titvinidze, Antonius Dorda, Wolfgang von der Linden, and Enrico Arrigoni — Institute of theoretical and computational physics, Graz Univeristy of Technology, 8010 Graz, Austria.

Here we investigate the effect of the interaction on the thermoelectric properties of a system, consisting of the single correlated layer sandwiched between two metallic leads. First we investigate linear response. We present our results for the seebeck coefficient, electrical and thermal conductance. Later on, we consider a finite temperature difference between the left and right leads. We study dependence of the current on the electronic filing of the central layer for zero bias voltage and current-voltage characteristics close to the half-filling. We obtain that strong interactions enhance thermoelectric effects, in both cases. Our results are obtained via non-equilibrium dynamical mean-field theory [1]. As an impurity solver we use auxiliary master equation approach [2], which addresses the impurity problem within an auxiliary system consisting of a correlated impurity, a small number of uncorrelated bath sites, and two Markovian environments described by a generalized master equation.

[1] P. Schmidt and H. Monien, ArXiv:cond-mat/0202046;
J. K. Freericks, Phys. Rev. B 77, 075109 (2008)
[2] E. Arrigoni et al, Phys. Rev. Lett. 110, 086403 (2013);
A. Dorda et al, Phys. Rev. B. 89, 165105 (2014);
I. Titvinidze et al., PRB 92, 245125 (2015)

15 min. break.

Invited Talk TT 62.7 Thu 11:15 HSZ 304

Optical Control of Complex Quantum Materials — •Stefan Kaiser — Max Planck Institut für Festkörperforschung und 4. Physikalisches Institut, Universität Stuttgart, Germany

Advanced ultrafast nonlinear optical methods open new ways of controlling complex solid-state materials on unprecedented timescales. In quantum materials, finding new ways of manipulating the complex interplay of electronic phases or effectively tuning electronic interactions opens new avenues in controlling physical properties and designing new functionalities. I will show how we investigate different scenarios like the balancing between competing phases triggered by ultrashort light pulses or possibilities of dynamical stabilization of new states of matter in periodically driven light fields. A remarkable effect are possibilities to induce superconductivity in high temperature cuprate superconductors at temperatures far above T_c [1-3]. Tuning local interactions [4,5] and possible light-induced superconductivity in the doped fullerides K_3C_{60} [6] will serve as important example that inducing such intriguing effects is a more general effect and not restricted to the rather specialized class of cuprate systems.

[1] D. Fausti et al. Science 331, 189 (2011)
[2] S. Kaiser et al. Phys. Rev. B 89, 184515 (2014)
[3] W. Hu et al. Nature Materials 13, 705 (2014)
[4] R. Singla et al. Phys. Rev Lett. 115, 187401 (2015)
[5] S. Kaiser et al. Sci. Rep. 4, 3823 (2014)
[6] M. Mitrano et al. Nature 530, 461 (2016)

TT 62.8 Thu 11:45 HSZ 304

Hund's exchange out of equilibrium — •Hugo Strand[1], Denis Golež[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 study the canonical model for strongly correlated Hund's metals, the two band Hubbard model with local density-density and Hund's exchange interaction. Using real-time dynamical mean-field theory and a first- and second-order strong coupling expansion impurity solver we find novel dynamical features as compared to the single band model. We study the Mott insulator at half-filling and the strong influence of the local doublon spin degrees of freedom on the relaxation dynamics after an excitation pulse.

TT 62.9 Thu 12:00 HSZ 304

Quantum Mutual Information as a Probe for Many-Body Localization — •Giuseppe De Tomasi, Soumya Bera, Jens Bardarson, and Frank Pollmann — MPI-PKS , Dresden Germany

We demonstrate that the quantum mutual information (QMI) is a useful probe to study many-body localization (MBL). First, we focus on the detection of a metal–insulator transition for two different models, the noninteracting Aubry-André-Harper model and the spinless fermionic disordered Hubbard chain. We find that the QMI in the localized phase decays exponentially with the distance between the regions traced out, allowing us to define a correlation length, which converges to the localization length in the case of one particle. Sec-

ond, we show how the QMI can be used as a dynamical indicator to distinguish an Anderson insulator phase from an MBL phase. By studying the spread of the QMI after a global quench from a random product state, we show that the QMI does not spread in the Anderson insulator phase but grows logarithmically in time in the MBL phase.

TT 62.10 Thu 12:15 HSZ 304

Quantum quenches in many-body localized systems — •Johannes Hauschild[1], Fabian Heidrich-Meisner[2], and Frank Pollmann[1] — [1]Fakultät für Physik, Technische Universität München, D-85748 Garching — [2]Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, D-80333 München

The field of many-body localization has recently attracted considerable theoretical and experimental interest. Many-body localized phases occur in interacting systems and are characterized by the absence of transport, the lack of thermalization, as well as the existence of quasi local integrals of motions. Ultra cold atoms have proven to be an ideal experimental test bed to test theoretical predictions. Most of the experiments involve the real time evolution of an initial state prepared by sudden changes in system parameters. First, we numerically investigate signatures of many-body localization by studying the melting of a domain wall after a quantum quench [1]. Second, we consider a dynamical system in which we couple initially hot and cold regions. We show that it is possible to extract characterizing properties like the localization length and the critical disorder strength.

[1] J. Hauschild et al., Phys. Rev. B 94, 161109(R)

TT 62.11 Thu 12:30 HSZ 304

Density propagator for many-body localization: finite size effects, transient subdiffusion, (stretched-)exponentials — •Soumya Bera[1], Giuseppe De Tomasi[1], Felix Weiner[2], and Ferdinand Evers[2] — [1]MPI-PKS, Dresden — [2]Institute of Theoretical Physics, University of Regensburg

We investigate charge relaxation in the spin-less disordered fermionic Hubbard chain (t–V-model). Our observable is the time-dependent density propagator, $\Pi_\varepsilon(x,t)$, calculated in windows of different energy density, ε, of the many-body Hamiltonian and at different disorder strengths, W, not exceeding the critical value W_c. The width $\Delta x_\varepsilon(t)$ of $\Pi_\varepsilon(x,t)$ exhibits a behavior $d\ln\Delta x_\varepsilon(t)/d\ln t{=}\beta_\varepsilon(t)$, where the exponent function $\beta_\varepsilon(t){\lesssim}1/2$ is seen to depend strongly on L at all investigated parameter combinations. (i) We confirm the existence of a region in phase space that exhibits subdiffusive dynamics in the sense that $\beta_\varepsilon(t){<}1/2$ in large window of times. However, subdiffusion might possibly be transient, only, finally giving way to a conventional diffusive behavior with $\beta_\varepsilon{=}1/2$. (ii) We cannot confirm the existence of many-body mobility edges deep in the delocalized phase. (iii) (Transient) subdiffusion $0<\beta_\varepsilon(t)\lesssim 1/2$, coexists with an enhanced probability for returning to the origin, $\Pi_\varepsilon(0,t)$, decaying much slower than $1/\Delta x_\varepsilon(t)$. Correspondingly, the spatial decay of $\Pi_\varepsilon(x,t)$ is far from Gaussian being exponential or even slower. On a phenomenological level, our findings are broadly consistent with effects of strong disorder and (fractal) Griffiths regions.

TT 62.12 Thu 12:45 HSZ 304

Occupation spectrum after a global quench in the many-body localized phase — Talía Lezama Mergold Love[1], Soumya Bera[1,3], and •Jens Hjorleifur Bardarson[1,2] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]Department of Theoretical Physics, KTH Royal Institute of Technology, Stockholm, SE-106 91 Sweden — [3]Department of Physics, IIT Bombay, India

Closed disordered interacting quantum systems can exhibit many-body localization (MBL). When disorder is sufficiently strong, such systems enter into a nonergodic regime known as the many-body localized phase, resulting in an ideal insulator with zero charge and thermal conductivities at finite energy densities. The emergent integrability of the MBL phase can be understood in terms of localized quasiparticles. As a result, the occupations of the one-particle density matrix (OPDM) in eigenstates show a fermi-liquid like discontinuity. In this work, we numerically explore the dynamics of the MBL phase generated by a global quench from a charge density state, in terms of the OPDM occupation spectrum. In particular, we show that in the steady state, the occupation discontinuity is smeared to a continuous distribution in a similar way as finite temperature smears the discontinuity in a fermi liquid, but the occupation spectrum remains highly non-thermal in the thermodynamic limit.

TT 63: Spincaloric Transport (joint session MA, TT, organized by MA)

Time: Thursday 9:30–12:00 Location: HSZ 403

TT 63.1 Thu 9:30 HSZ 403

Tunnel magneto-Seebeck effect in $MgAl_2O_4$ based magnetic tunnel junctions — •Torsten Huebner[1], Alexander Boehnke[1], Ulrike Martens[2], Andy Thomas[3], Günter Reiss[1], Markus Münzenberg[2], and Timo Kuschel[1,4] — [1]CSMD, Physics Department, Bielefeld University, Germany — [2]IFP, Greifswald University, Germany — [3]IMW, IFW Dresden, Germany — [4]University of Groningen, The Netherlands

The tunnel magneto-Seebeck (TMS) effect describes the changing Seebeck coefficient of a magnetic tunnel junction (MTJ) depending on the relative magnetization alignment of its ferromagnetic electrodes. This effect has been measured in several material systems and with different experimental methods [1-4]. In our study, we focus on MTJs with $MgAl_2O_4$ (MAO) barrier, because of its theoretical advantages in comparison to MgO [5,6]. We find a distinct maximum of the TMS effect at a nominal barrier thickness of 2.6 nm, almost doubling the effect ratio measured at standard barrier thicknesses of (1.8-2.0) nm.

[1] Walter et al., Nat. Mater. 10, 742 (2011)
[2] Liebing et al., Phys. Rev. Lett. 107, 177201 (2011)
[3] Boehnke et al., Rev. Sci. Instrum. 84, 063905 (2013)
[4] Huebner et al., Phys. Rev. B 93, 224433 (2016)
[5] Zhang et al., Appl. Phys. Lett. 100, 222401 (2012)
[6] Miura et al., Phys. Rev. B 86, 024426 (2012)

TT 63.2 Thu 9:45 HSZ 403

Quantitative disentanglement of spin Seebeck, intrinsic anomalous Nernst, and proximity-induced anomalous Nernst effect in NM/FM bilayers — •Panagiota Bougiatioti[1], Christoph Klewe[1,2], Daniel Meier[1], Orestis Manos[1], Olga Kuschel[3], Joachim Wollschläger[3], Laurence Bouchenoire[4,5], Simon D. Brown[4,5], Jan-Michael Schmalhorst[1], Günter Reiss[1], and Timo Kuschel[1,6] — [1]CSMD, Physics Department, Bielefeld University, Germany — [2]ALS, Berkeley, California, USA — [3]Fachbereich Physik, Universität Osnabrück, Germany — [4]XMaS, ESRF, Grenoble, France — [5]University of Liverpool, UK — [6]University of Groningen, The Netherlands

In this project, we investigate thermal transport phenomena by separating the anomalous Nernst effect (ANE) contribution (intrinsic and proximity-induced) from the spin Seebeck effect (SSE) voltage on sputter-deposited $Pt/NiFe_2O_{4-x}$ samples. On one hand, we observe a distinct increase of the SSE with the increase of the bandgap energy and the decrease of conductivity, whereas the ANE decreases. On the other hand, a proximity-induced ANE could only be identified in the metallic $Pt/Ni_{33}Fe_{67}$ bilayer. This was verified by the investigation of static magnetic proximity effects via x-ray resonant magnetic reflectivity [1-3]. Further, we determined a maximum moment of 0.48 μ_B per spin-polarized Pt atom in the $Pt/Ni_{33}Fe_{67}$ bilayer.

TT 63.3 Thu 10:00 HSZ 403

Magneto-Seebeck Tunneling Across a Vacuum Barrier — •Cody Friesen, Hermann Osterhage, and Stefan Krause — Department of Physics, University of Hamburg, Jungiusstr. 11A, 20355 Hamburg, Germany

The tunneling magneto-Seebeck effect has been intensively studied both for its potential applications in e.g. waste heat recycling in electronics, and for the insights it can provide into fundamental solid state phenomena [1]. Previously, spin-resolved measurements have been performed using planar magnetic tunneling junctions [2], which limits the achievable spatial resolution.

We have investigated (magneto-)Seebeck tunneling across a vacuum

barrier using spin-polarized scanning tunneling microscopy (SP-STM) [4], at low temperatures ($T = 50\,\mathrm{K}$) and UHV conditions. A 15 mW fiber-coupled diode laser was used to heat only the magnetic STM tip, creating a controllable temperature differential across the junction. With this approach the contribution of different surfaces to magneto-Seebeck tunneling has been probed on the Fe/W(110) monolayer system. The first laterally resolved experimental results will be shown and discussed in terms of tunneling thermovoltage and associated magneto-Seebeck coefficients.

[1] G. Bauer *et al.*, Nat. Mater. **11**, 5 (2012).
[2] M. Walter *et al.*, Nat Mater **10**, 10 (2011).
[3] R. Wiesendanger, Rev. Mod. Phys. **81**, 4 (2009).

TT 63.4 Thu 10:15 HSZ 403

Interface dependent magnon mode coupling in insulating ferrimagnets — •Joel Cramer[1,2], Er-Jia Guo[1,3], Andreas Kehlberger[1], Gerhard Jakob[1], and Mathias Kläui[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz, 55128 Mainz, Germany — [3]Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, 37830 TN, USA

One of the contemporary challenges of magnon spintronics is the profound understanding of magnon mode dependent transport and interface transmission. To approach this problem, we present temperature dependent spin Seebeck (SSE) measurements in uncompensated (yttrium iron garnet (YIG) [1]) and compensated (e.g. gadolinium iron garnet (GdIG) [2]) insulating ferrimagnets. In YIG, a giant enhancement of the SSE amplitude is observed at low temperatures. Despite the bulk origin of the spin current generation, the temperature dependence varies with the used heavy metal (HM) detection layer. Systematic studies including transmission electron microscopy (TEM) reveal that this effect is due to the altered atomistic composition of YIG at the interface. In compensated ferrimagnets, the opposite contribution of distinct magnon modes leads to a sign change of the spin current at low temperatures [3]. We show that different HM layers as well as a modified GdIG surface morphology result in varied interface couplings of these modes, expressed by a temperature shift of the sign change.
[1] Guo et al., Phys. Rev. X 3, 031012 (2016) [2] Cramer et al., (under review) [3] Geprägs et al., Nature Comm. 7, 10452 (2016)

TT 63.5 Thu 10:30 HSZ 403

Quantitative disentanglement of spin Seebeck, intrinsic anomalous Nernst, and proximity-induced anomalous Nernst effect in NM/FM bilayers — •Panagiota Bougiatioti[1], Christoph Klewe[1,2], Daniel Meier[1], Orestis Manos[1], Olga Kuschel[3], Joachim Wollschläger[3], Laurence Bouchenoire[4,5], Simon D. Brown[4,5], Jan-Michael Schmalhorst[1], Günter Reiss[1], and Timo Kuschel[1,6] — [1]CSMD, Physics Department, Bielefeld University, Germany — [2]ALS, Berkeley, California, USA — [3]Fachbereich Physik, Universität Osnabrück, Germany — [4]XMaS, ESRF, Grenoble, France — [5]University of Liverpool, UK — [6]University of Groningen, The Netherlands

In this project, we investigate thermal transport phenomena by separating the anomalous Nernst effect (ANE) contribution (intrinsic and proximity-induced) from the spin Seebeck effect (SSE) voltage on sputter-deposited Pt/$NiFe_2O_{4-x}$ samples. On one hand, we observe a distinct increase of the SSE with the increase of the bandgap energy and the decrease of conductivity, whereas the ANE decreases. On the other hand, a proximity-induced ANE could only be identified in the metallic Pt/$Ni_{33}Fe_{67}$ bilayer. This was verified by the investigation of static magnetic proximity effects via x-ray resonant magnetic reflectivity [1-3]. Further, we determined a maximum moment of 0.48 μ_B per spin-polarized Pt atom in the Pt/$Ni_{33}Fe_{67}$ bilayer.
[1] T. Kuschel et al., Phys. Rev. Lett. 115, 097401 (2015)
[2] T. Kuschel et al., IEEE Trans. Magn. 52, 4500104 (2016)
[3] C. Klewe et al., Phys. Rev. B 93, 214440 (2016)

15 min. break.

TT 63.6 Thu 11:00 HSZ 403

Pumping laser excited spins through MgO barriers — •Ulrike Martens[1], Jakob Walowski[1], Thomas Schumann[1], Maria Mansurova[1], Alexander Boehnke[2], Torsten Huebner[2], Guenter Reiss[2], Andy Thomas[3], and Markus Muenzenberg[1] — [1]Institut für Physik, EMAU Greifswald, Germany — [2]CSMD, Physics Department, Bielefeld University, Germany — [3]Institute for Metallic Materials, IFW Dresden, Germany

We present a study of the tunnel magneto-Seebeck (TMS) effect in MgO based magnetic tunnel junctions (MTJs). The electrodes consist of CoFeB with in-plane magnetic anisotropy. The temperature gradients which generate a voltage across the MTJs layer stack are created using laser heating. Using this method, the temperature can be controlled on the micrometer length scale: here, we investigate, how both, the TMS voltage and the TMS effect, depend on the size, position and intensity of the applied laser spot. For this study, a large variety of different temperature distributions was created across the junction. We recorded two-dimensional maps of voltages generated by heating in dependence of the laser spot position and the corresponding calculated TMS values. The voltages change in value and sign, from large positive values when heating the MTJ directly in the centre to small values when heating the junction on the edges and even small negative values when heating the sample away from the junction. Those zero crossings lead to very high calculated TMS ratios.
Funding by DFG SPP 1538 is acknowledged

TT 63.7 Thu 11:15 HSZ 403

Thermally Induced Spin Transfer Torque on MgO-based magnetic tunnel junctions using microresonators — •Hamza Cansever[1,2], Ciaran Fowley[1], Rysard Narkovicz[1], Ewa Kowalska[1,2], Yuriy Aleksandrov[2], Oguz Yildirim[1], Aleksandra Titova[1,2], Kilian Lenz[1], Jürgen Lindner[1], Jürgen Fassbende[1], and Alina M. Deac[1] — [1]Helmholtz Zentrum Dresden Rossendorf Institute of Ion Beam Physics and Materials Research — [2]TU Dresden Institute of Solid State Physics

Magnetic tunnel junctions have been commonly used in spintronics applications, such as magnetic random access memory (M-RAM), spin transfer torque RAM (STT-RAM) and hard disc drive (HDD) because of high storage capacity. A spin polarized current flowing through a ferromagnetic layer can exert spin-transfer-torque (STT) on the local magnetization. When we apply thermal gradient across the junction we can induce what is called thermal spin transfer torque (T-STT). In this study, the microresonator FMR technique is used in order to analyze how the ferromagnetic resonance signal corresponding to the free layer of an in-plane MgO-based tunnel junction device is modified in the presence of a temperature gradients across the barrier. Details of resonator fabrication and preliminary measurements are presented.
This work is supported by DFG-SPP1538.

TT 63.8 Thu 11:30 HSZ 403

Quantitative separation of the anisotropic magnetothermopower and planar Nernst effect by the rotation of an in-plane thermal gradient — •Oliver Reimer[1], Daniel Meier[1], Michel Bovender[1], Lars Helmich[1], Jan-Oliver Dreessen[1], Jan Krieft[1], Jan-Michael Schmalhorst[1], Andreas Hueutten[1], Guenter Reiss[1], and Timo Kuschel[1,2] — [1]CSMD, Physics Department, Bielefeld University, Germany — [2]University of Groningen, The Netherlands

A ferromagnet exposed to a thermal gradient ∇T in an external magnetic field $\vec{H}$ generates a spin current parallel to ∇T (longitudinal spin Seebeck effect [1]) which can be detected in materials with high spin orbit coupling (e.g. Pt) by the inverse spin Hall effect. Up to now, all spin caloric experiments employ a spatially fixed ∇T. The use of a recently reported new experimental setup allows the rotation of an in-plane ∇T [2]. In this talk, it will be shown, that combined with a rotatable external magnetic field, the rotation of ∇T reveals a phase shift of the magnetothermopower angular dependence with respect to the magnetization direction in a permalloy thin film. Supported by a theoretical model this phase shift allows to unambiguously separate the Seebeck voltage, the anisotropic magnetothermopower and the planar Nernst effect within one experiment.
[1] K. Uchida et al., Appl. Phys. Lett. 97, 172505 (2010)
[2] O. Reimer et al., arXiv: 1609.08822 (2016)

TT 63.9 Thu 11:45 HSZ 403

Insights into the spin-orbit coupling mediated thermoelectric properties of half metallic full Heusler alloys — •Voicu Popescu and Peter Kratzer — Faculty of Physics and CENIDE, University Duisburg-Essen, 47057 Duisburg, Germany

We have performed first-principles investigations on the native defects in the half-metallic ferromagnetic full Heusler alloys Co$_2$TiZ (Z one of the group IV elements Si, Ge, Sn). We modelled the defects as dilute alloys, and treated them in the coherent potential approximation within the framework of the full potential spin-polarized relativistic Korringa-Kohn-Rostoker Green function method. The self-

consistent potentials determined this way were used to calculate the residual resistivity via the Kubo-Greenwood formula and, based on its energy dependence, the Seebeck coefficient of the systems. The latter is shown to depend significantly on the type of defect, variations that are related to subtle changes in the electronic structure around the half-metallic gap induced by the spin-orbit coupling. Amongst the different investigated intrinsic defects, two of them exhibit a negative Seebeck coefficient, in good agreement with the available experimental data.

TT 64: Coherent Quantum Dynamics (joint session DY, TT, organized by DY)

Time: Thursday 9:30–13:15 Location: ZEU 160

Invited Talk TT 64.1 Thu 9:30 ZEU 160

Equilibration and ensembles in coherent quantum systems — •Fabian Essler — Oxford University

I consider the relaxation after quantum quenches in isolated quantum systems. In the thermodynamic limit local relaxation towards a stationary state occurs. I first discuss the characterization of the stationary state for generic and integrable systems and how this relates to properties of finite energy density eigenstates. In generic systems the stationary state is locally thermal and has a volume-law entanglement entropy, while there is a considerably richer set of possibilities in integrable models. I then turn to the recently proposed "quantum disentangled liquid", in which thermalized and non-thermalized degrees of freedom are postulated to co-exist. I discuss the possible existence of such states in the half-filled Hubbard model with strong repulsive interactions.

TT 64.2 Thu 10:00 ZEU 160

Thermalization and light cones in a model with weak integrability breaking — Bruno Bertini[1,2], Fabian Essler[1], •Stefan Groha[1], and Neil Robinson[3] — [1]The Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, OX1 3NP, United Kingdom — [2]SISSA and INFN, Sezione di Trieste, via Bonomea 265, I-34136, Trieste, Italy — [3]Condensed Matter Physics and Materials Science Division, Brookhaven National Laboratory, Upton, New York 11973, USA

We employ equation of motion techniques to study the non-equilibrium dynamics in a lattice model of weakly interacting spinless fermions. Our model provides a simple setting for analyzing the effects of weak integrability breaking perturbations on the time evolution after a quantum quench. For sufficiently weak integrability-breaking interactions we always observe prethermalization plateaux, where local observables relax to non-thermal values at intermediate time scales. At later times a crossover towards thermal behaviour sets in. We determine the associated time scale, which depends on the initial state, the band structure of the non-interacting theory, and the strength of the integrability breaking perturbation. Our method allows us to analyze in some detail the spreading of correlations and in particular the structure of the associated light cones in our model. We find that the interior and exterior of the light cone are separated by an intermediate region, the temporal width of which appears to scale with a universal power-law $t^{1/3}$.

TT 64.3 Thu 10:15 ZEU 160

Non-equilibrium interacting integrable models — •Jacopo De Nardis[1], Jean-Sébastien Caux[2], Enej Ilievski[2], Michael Brockmann[3], and Milosz Panfil[4] — [1]CNRS-Laboratoire de Physique Théorique de l'Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex, France — [2]Institute for Theoretical Physics, University of Amsterdam, Science Park 904,
Postbus 94485, 1090 GL Amsterdam, The Netherlands — [3]Max Planck Institute for the Physics of Complex Systems, Nothnitzer Str. 38, 01187 Dresden, Germany — [4]Institute of Theoretical Physics, University of Warsaw,
ul. Pasteura 5, 02-093 Warsaw, Poland.

We review the recent progresses in computing the non-equilibrium steady states (often referred as Generalized Gibbs Ensemble states) of interacting integrable models, as the XXZ spin 1/2 chain and the Lieb-Liniger model for interacting bosons on a line. We show how the role of quasi-local charges is fundamental in order to capture the long time limit of the expectation values of simple local observables and how important information regarding the time evolution towards equilibrium can be extracted by such steady states and their thermodynamic quasi-particle excitations. Finally we show how the steady state can be directly computed via experimental observations with cold atoms in a shallow trap or in an optical lattice.

TT 64.4 Thu 10:30 ZEU 160

Quenching a Quantum Critical State by the Order Parameter: Dynamical Quantum Phase Transitions and Quantum Speed Limits — •Markus Heyl — Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany

Quantum critical states exhibit strong quantum fluctuations and are therefore highly susceptible to perturbations. In this work we study the dynamical stability against a sudden coupling to these strong fluctuations by quenching the order parameter of the underlying transition. We find that such a quench can generate superextensive energy fluctuations. This leads to a dynamical quantum phase transition with nonanalytic real-time behavior in the resulting decay of the initial state. At the corresponding critical time the dynamically-evolved state becomes orthogonal to the initial one yielding an unconventional quantum speed limit. An outlook is given on the implications onto potential restricted thermalization despite of nonintegrability.

TT 64.5 Thu 10:45 ZEU 160

Localization in a disorder-free model after a global quantum quench. — •Adam Smith[1], Johannes Knolle[1], Dmitry Kovrizhin[2], and Roderich Moessner[3] — [1]T.C.M. group, Cavendish Laboratory, JJ Thomson Ave, Cambridge CB3 0HE, United Kingdon — [2]Rudolf Peierls Centre for Theoretical Physics, 1 Keble Road, Oxford OX1 3NP, United Kingdom — [3]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany

We consider an interacting, translation invariant one dimensional model in which we observe complete localisation in one of two fermionic subsystems. Its effective disorder is generated dynamically and can be rigorously identified through a set of conserved quantities. To corroborate the emergence of localization after a global quantum quench we show persistence of a density wave in the initial state, absence of domain-wall melting, and suppression of light-cone growth of correlations.

TT 64.6 Thu 11:00 ZEU 160

Transport in Out-of-Equilibrium XXZ Chains: Exact Pro les of Charges and Currents — •Bruno Bertini[1], Mario Collura[1,2], Jacopo De Nardis[3], and Maurizio Fagotti[3] — [1]SISSA and INFN, Trieste, Italy — [2]Oxford University, Oxford, United Kingdom — [3]École normale supérieure, Paris, France

We consider the non-equilibrium time evolution of piecewise homogeneous states in the XXZ spin-1/2 chain, a paradigmatic example of an interacting integrable model. The initial state can be thought as the result of joining chains with different global properties. Through dephasing, at late times the state becomes locally equivalent to a stationary state which explicitly depends on position and time. We propose a kinetic theory of elementary excitations and derive a continuity equation which fully characterizes the thermodynamics of the model. We restrict ourselves to the gapless phase and consider cases where the chains are prepared: 1) at different temperatures; 2) in the ground state of two different models; 3) in the "domain wall" state. We find excellent agreement (any discrepancy is within the numerical error) between theoretical predictions and numerical simulations of time evolution based on TEBD algorithms. As a corollary, we unveil an exact expression for the expectation values of the charge currents in a generic stationary state.

15 min. break

TT 64.7 Thu 11:30 ZEU 160

Unconventional quasienergy bands in tilted optical lattices — •Onno Renke Diermann — Institut für Physik, Carl von Ossietzky

Universität Oldenburg

The existence of quasienergy bands in periodically driven lattices under the influence of an additional static force has first been predicted by J.Zak ["Finite Translations in Time and Energy", Phys. Rev. Lett **71**, 2624 (1993)]. Among other things, it was suggested that within a single-band approximation such bands may take the form of cosine bands "modulated with the Bessel function of the shaking amplitude". Considering the experimentally accessible example of ultracold atoms in deep shaken cosine lattices, we show by numerical calculations of the full quasienergy spectrum that the single-band approximation is not reliable, and the quasienergy bands in fact are broken by a multitude of multiphoton resonances. This means that particles prepared in such bands tend to heat up on short time scales, and dynamic localization will be hard to observe.

TT 64.8 Thu 11:45 ZEU 160

iDMRG Study of the Kitaev-Heisenberg Model — •Matthias Gohlke, Ruben Verresen, Frank Pollmann, and Roderich Moessner — MPI-PKS, Dresden, Germany

Quantum spin-liquids represent novel phases of matter that host emergent fractionalized excitations. The Kitaev-Heisenberg model is a two-dimensional model system in this context and relevant for recent experiments on putative quantum spin-liquid materials. We revisit the ground state phase diagram of the Kitaev-Heisenberg model using large scale infinite density-matrix renormalization group method of cylinders with up to twelve sites circumference. In particular, the cylindrical geometry allows to capture the gapless points and to extract its universal critical properties. Furthermore, we observe that the gapless excitations remain stable under perturbation with Heisenberg interaction.

TT 64.9 Thu 12:00 ZEU 160

Dynamics of the Kitaev-Heisenberg Model — •Ruben Verresen, Matthias Gohlke, Roderich Moessner, and Frank Pollmann — MPI for Physics of Complex Systems, Dresden, Germany

Quantum spin-liquids represent novel phases of matter that host emergent fractionalized excitations. The Kitaev-Heisenberg model is a two-dimensional model system in this context and relevant for recent experiments on putative quantum spin-liquid materials. We obtain the dynamical spin-structure factor for this model using a matrix-product state based method. This quantity can be compared to neutron scattering measurements and provides characteristic insights into the dynamics of the fractionalized excitations. We find significant broad high energy features beyond spin-wave theory even in the ordered phases when tuned near the spin-liquid regime. We then focus on the zig-zag phase of the Kitaev-Heisenberg model which is relevant for α-$RuCl_3$ and observe that the high energy part reveals features that were first seen in neutron scattering experiments, displaying proximate spin liquid physics. In particular we are led to the interpretation of the observed broad high energy features as the intersection of remnants of very diffuse spin-wave bands.

TT 64.10 Thu 12:15 ZEU 160

Probing density and spin correlations in two-dimensional Hubbard model with ultracold fermions — •Chun Fai Chan[1], Jan Henning Drewes[1], Marcell Gall[1], Nicola Wurz[1], Eugenio Cocchi[1,2], Luke Miller[1,2], Daniel Pertot[1], Ferdinand Brennecke[1], and Michael Köhl[1] — [1]Physikalisches Institut, University of Bonn, Wegelerstrasse 8, 53115 Bonn, Germany — [2]Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Quantum gases of interacting fermionic atoms in optical lattices is a promising candidate to study strongly correlated quantum phases of the Hubbard model such as the Mott-insulator, spin-ordered phases, or in particular d-wave superconductivity. We experimentally realise the two-dimensional Hubbard model by loading a quantum degenerate Fermi gas of 40K atoms into a three-dimensional optical lattice geometry. High-resolution absorption imaging in combination with radiofrequency spectroscopy is applied to spatially resolve the atomic distribution in a single 2D layer. We investigate in local measurements of spatial correlations in both the density and spin sector as a function of filling, temperature and interaction strength. In the density sector, we compare the local density fluctuations and the global thermodynamic quantities, and in the spin sector, we observe the onset of non-local spin correlation, signalling the emergence of the anti-ferromagnetic phase.

TT 64.11 Thu 12:30 ZEU 160

Adiabatic Dynamics of the Excited States for the Lipkin-Meshkov-Glick Model — •Wassilij Kopylov and Tobias Brandes — Technische Universität Berlin, Institut für Theoretische Physik, Berlin, Deutschland

We theoretically investigate the impact of the excited state quantum phase transition (ESQPT) on the adiabatic dynamics for the Lipkin-Meshkov-Glick model. Using a time dependent protocol, we continuously change a model parameter and discuss then the scaling properties of the system especially close to the ESQPT. On top, we show that the mean-field dynamic with the time dependent protocol gives the correct expectation values in the thermodynamic limit even for the excited states.

1) W. H. Zurek, U. Dorner, and P. Zoller, PRL 95, 105701 (2005)
2) H. J Lipkin, N. Meshkov and A. Glick, Nucl. Phys. 62, 188 (1965)
3)T. Caneva, R. Fazio and G. E. Santoro, PRB 78, 104426 (2008)

TT 64.12 Thu 12:45 ZEU 160

Spectral functions of quantum impurity models in the long-time limit of the time-dependent numerical renormalization group approach — •Theo Costi and Hoa Nghiem — Peter Grünberg Institut (PGI-2) and Institute for Advanced Simulation IAS-3), Forschungszentrum Jülich, Jülich, Germany

We develop a new multiple-quench time dependent numerical renormalization group (TDNRG) approach to study the time-evolution of strongly correlated quantum impurities in response to quantum quenches, pulses and periodic driving fields with potential application to a number of fields, including cold atom systems, non-equilibrium transport in nanoscale devices, and the theory of pump-probe spectroscopies of correlated materials within the non-equilibrium dynamical mean field theory. While the single-quench TDNRG suffers from sizeable errors for spectral functions and thermodynamic observables in the long-time limit, we show that our new multiple-quench TDNRG approach systematically reduces these errors to negligible values. Precise results are presented for local observables of the Anderson model, both static (local occupation and double occupancy) and dynamic (spectral function), in the long-time limit. For finite times and periodic driving, we demostrate a significant improvement for the time evolution of the local occupation as compared to our previous approach [1].

[1] H. T. M. Nghiem, T. A. Costi, Phys. Rev. B90, 035129 (2014).

TT 64.13 Thu 13:00 ZEU 160

Energy exchange in driven open quantum systems at strong coupling — •Matteo Carrega[1], Paolo Solinas[2], Maura Sassetti[2,3], and Ulrich Weiss[4] — [1]Nest, Istituto Nanoscienze and Scuola Normale Superiore (CNR-Pisa) — [2]SPIN-CNR — [3]Università di Genova — [4]Universität Stuttgart

The time-dependent energy transfer in a driven quantum system strongly coupled to a heat bath is studied within an influence functional approach. Exact formal expressions for the statistics of energy dissipation into the different channels are derived. The general method is applied to the driven dissipative two-state system. It is shown that the energy flows obey a balance relation, and that, for strong coupling, the interaction may constitute the major dissipative channel. Results in analytic form are presented for the particular value K = 1/2 strong Ohmic dissipation. The energy flows show interesting behaviors including driving-induced coherences and quantum stochastic resonances. It is found that the general characteristics persists for K near 1/2.

TT 65: Topological Insulators I (joint session DS, HL, MA, O, TT, organized by HL)

Time: Thursday 9:30–12:45 Location: POT 251

Invited Talk TT 65.1 Thu 9:30 POT 251

Sub-nm probing of Topological insulators and Rashba systems — •Markus Morgenstern — II. Institute of Physics and JARA-FIT, RWTH Aachen, D-52074 Aachen, Germany

Spin-orbit interactions in solids are the key for many anticipated new functionalities ranging from the meanwhile traditional Datta-Das transistor to topological quantum computation using Majorana excitations. Local probes can provide crucial information on this interaction down to the nm scale. Within this talk, I will show how scanning tunneling spectroscopy reveals the presence of topologically protected edge states provided by a spin-orbit induced band inversion of heavy metal graphene [1], how the detrimental fluctuations of the spin-orbit interaction can be probed down to the nm length scale [2], and that ferroelectricity induces Rashba-type spin-orbit interaction within the bulk of the simple binary material GeTe [3].

[1] C. Pauly et al., Nat. Phys. 11, 338 (2015); ACS Nano 10, 3995 (2016). [2] J. R. Bindel et al., Nat. Phys. 12, 920 (2016). [3] M. Liebmann et al., Adv. Mat. 20, 560 (2016); H. J. Elmers et al., Phys. Rev. B 94, 201403 (2016).

TT 65.2 Thu 10:00 POT 251

2D Topological Insulators: Trends in Chemical Space — •Carlos Mera Acosta[1,2], Christian Carbogno[1], Adalberto Fazzio[2], Luca M. Ghiringhelli[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Instituto de Física, Universidade de São Paulo, SP, Brazil

2D topological insulators (TI) have attracted considerable scientific interest in recent years [1]. The search for new TIs has often focused on elements with strong spin-orbit coupling (SOC) [2], which can induce the necessary topological transition. In this work, we have computed the topological invariant Z_2 for 200 functionalized honeycomb-lattice systems using our recent Wannier center of charge (WCC) [3] implementation in the FHI-aims electronic structure code. Besides confirming the TI character of well-known materials, e.g., functionalized stanene [1], our study found several other yet unreported TIs. This reveals that also elements with relatively low SOC can form TIs. To analyze the observed trends in chemical space we relate the WCCs to the atomic features of the constituent atoms using a compressed-sensing approach. For this purpose, the LASSO and ℓ_0 minimization of Ref. [4] is extended from learning scalar properties to functions.

This work received funding from The Novel Materials Discovery (NOMAD) Laboratory, a European Centre of Excellence.

[1] Y. Ren, Z. Qiao, and Q. Niu, *RPP* **79**, 6 66501 (2016).
[2] M. Z. Hasan and C. L. Kane, *Rev. Mod. Phys.* **82**, 3045 (2010).
[3] R. Yu, *et al.*, *Phys. Rev. B* **84**, 075119 (2011).
[4] L. M. Ghirighelli, *et al.*, *Phys. Rev. Lett.* **114**, 105503 (2015).

TT 65.3 Thu 10:15 POT 251

Occupied topological surface states in strained α-Sn — Victor Rogalev[1], •Tomáš Rauch[2], Markus Scholz[1], Felix Reis[1], Lenart Dudy[1], Andrzej Fleszar[3], Vladimir Strocov[4], Jürgen Henk[2], Ingrid Mertig[2,5], Jörg Schäfer[1], and Ralph Claessen[1] — [1]Physikalisches Institut und Röntgen Center for Complex Material Systems, Universität Würzburg, 97074 Würzburg, Germany — [2]Institute of Physics, Martin Luther University Halle-Wittenberg, 06099 Halle (Saale), Germany — [3]Institut für Theoretische Physik und Astronomie, Universität Würzburg, 97074 Würzburg, Germany — [4]Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen, Switzerland — [5]Max Planck Institute for Microstructure Physics, 06120 Halle (Saale), Germany

Unstrained α-Sn is a semimetal with a non-trivial band ordering at the Γ point of the bulk Brillouin zone: $E(\Gamma_8^+) > E(\Gamma_7^-) > E(\Gamma_7^+)$. Strain in (001) direction lifts the degeneracy of the Γ_8^+ level at the Fermi energy. We demonstrate that compressive strain turns the system into a strong topological insulator, whereas tensile strain causes a transition into the topological Dirac semimetal phase.

I will present the results of calculations carried out along experimental findings obtained by soft X-ray angle-resolved photoemission. I will show that the existence of a previously unknown surface state located in the occupied projected bulk band structure of α-Sn is unveiled by both experimental and theoretical methods. In addition, its topological origin was confirmed by calculating the topological invariants of the bulk bands.

TT 65.4 Thu 10:30 POT 251

Engineering topological phases in crystalline symmetry-protected monolayers — •Chengwang Niu, Patrick M. Buhl, Gustav Bihlmayer, Daniel Wortmann, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The properties that distinguish topological crystalline insulators (TCIs) and topological insulators (TIs) rely on crystalline symmetry and time-reversal symmetry, respectively, which encodes different surface/edge properties. Here, we predict theoretically that TlM, thallium chalcogenide, (M = S and Se) (110) monolayers realize a family of two-dimensional (2D) TCIs characterized by mirror Chern number $\mathcal{C}_M = -2$ with an even number of band inversions. [1] Remarkably, under uniaxial strain ($\approx 1\%$), a topological phase transition between 2D TCI and 2D TI is revealed in TlM. In contrast, for Na_3Bi, the band inversion occur at single k point, thus a coexistence of 2D TI and 2D TCI is obtained. [2] Finally, we show different edge-state behaviors, especially at the time reversal invariant points.

This work was supported by SPP 1666 of the DFG.

[1] C. Niu, P. M. Buhl, G. Bihlmayer, D. Wortmann, S. Blügel, and Y. Mokrousov, Nano Lett. **15**, 6071 (2015).
[2] C. Niu, P. M. Buhl, G. Bihlmayer, D. Wortmann, S. Blügel, and Y. Mokrousov, submitted.

TT 65.5 Thu 10:45 POT 251

Anisotropy of Magneto-Transport on the Surface of Topological Insulators — •Alexey Taskin[1], Henry Legg[2], Fan Yang[1], Andrea Bliesener[1], Satoshi Sasaki[3], Yasushi Kanai[3], Kazuhiko Matsumoto[3], Achim Rosch[2], and Yoichi Ando[1] — [1]Institute of Physics II, University of Cologne — [2]Institute for Theoretical Physics, University of Cologne — [3]Scientific and Industrial Research, Osaka University

Recent advances in MBE growth and microfabrication technique allow to obtain Topological Insulator (TI) systems where the transport is dominated by the surface. Here we report a magneto-transport study of high-quality bulk-insulating $Bi_{2-x}Sb_xTe_3$ thin films, which were fabricated into devices with electrostatic gates on both bottom and top surfaces. For magnetic fields applied parallel to the surface of a TI, we found a clear anisotropy in magnetoresistance and related planar Hall effect that originates from the fundamental property of the surface Dirac fermions, the locking of their spin and momentum. The key signature of anisotropic magnetoresistance is a strong dependence on the gate voltage with a characteristic two-peak structure near the Dirac point. The observed anisotropy is related to a modification of the topological protection of the Dirac electrons against backscattering from impurities in the in-plane magnetic field and provides an example of a controllable time-reversal breaking on the surface of TIs.

Coffee Break

TT 65.6 Thu 11:30 POT 251

Topological insulator - superconductor hybrid devices — •Peter Schüffelgen, Daniel Rosenbach, Michael Schleenvoigt, Tobias W. Schmitt, Martin Lanius, Christian Weyrich, Tristan Heider, Benjamin Bennemann, Stefan Trellenkamp, Elmar Neumann, Gregor Mussler, Thomas Schäpers, and Detlev Grützmacher — Peter Grünberg Institute 9, Forschungszentrum Jülich & JARA-FIT, 52425 Jülich, Germany

3D topological insulators (TIs) possess metallic surface states with a spin-locked momentum. Therefore, in proximity to an s-wave superconductor, Majorana zero modes (MZMs) are predicted to occur at the surface of TIs. We found first signatures of 4π-periodic Josephson supercurrents in our topological Josephson junctions. The TI thin film was grown by means of molecular beam epitaxy on a Si(111) substrate and capped in-situ by a thin layer of aluminum to prevent thin film degradation and to preserve the pristine surface states during ex-situ fabrication. To increase the 4π-periodic contribution we fabricated quasi 1D Josephson junctions on pre-patterned silicon substrates. By covering the Si-111 surface partly with a thin layer of Si3N4/SiO2 we

made the topological insulator grow only on the silicon surface. In this way we were able to realize 1D trenches by predefining the MESA structure before MBE growth. To further improve the quality of our hybrid devices we developed a process, which allows to deposit superconducting contacts via stencil lithography. Combining this technique with selective area growth allows to fabricate complex devices in-situ.

TT 65.7 Thu 11:45 POT 251

Ultrafast mid-IR pump, THz probe spectroscopy investigating of the topological insulator BSTS — •Matteo Montagnese, Jingy Zhu, Chris Rheinhoffer, Yoichi Ando, and Paul H. M. van Loosdrecht — II. Physikalishes Institut der Universität zu Köln, Zülpicher str 77, D-25127 Köln

We present ultrafast pump-probe measurements on the topological insulator BSTS. We employed a high-intensity tunable mid-IR pulse (2-10 microns) as a pump, generated by difference-frequency mixing in an optical parametric amplifier to excite the BSTS system below the onset of the bulk optical electronic continuum. Upon excitation, the far-IR (0.1-3 THz) response of the system has been probed by a single-cycle coherent THz pulse, generated by optical rectification of a near-IR pulse. The time-resolved transmittance of the THz spectra have been measured employing optical sampling and time-domain techniques. By tuning the pump energy, the impurity states leading to charge puddle formation and the surface state are selectively populated, with the aim of disentangling their respective contributions to the dynamic optical conductivity.

TT 65.8 Thu 12:00 POT 251

Observation of the Quantum Anomalous Hall Effect depending on structural properties of $(VBiSb)_2Te_3$ layers — •Martin Winnerlein, Steffen Schreyeck, Stefan Grauer, Sabine Rosenberger, Kajetan Fijalkowski, Charles Gould, Karl Brunner, and Laurens W. Molenkamp — Physikalisches Institut, Experimentelle Physik III, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The quantum anomalous Hall effect is observed in thin V-doped $(BiSb)_2Te_3$ layers, a magnetic topological insulator. Thin layers revealing quantization are reproducibly deposited by molecular beam epitaxy at growth conditions effecting a compromise between controlled layer properties and high crystal quality. The influence of Sb content, layer thickness, structural quality, used substrates and cap layers is studied.

The Sb content is the main layer parameter to be optimized in order to approach charge neutrality. The Sb content is reliably determined from the in-plane lattice constant measured by X-ray diffraction even in thin layers. Within a narrow range at about 80% Sb content, the Hall resistivity reveals a maximum at 4 K and quantizes at mK temperatures [1]. Under these conditions thin layers grown on Si(111) or InP(111) and with or without a Te cap layer exhibit quantization. The quantization persists independently from the substrate, cap layer, the limited crystal quality and the degradation of the layer. This proves the robustness of the quantum anomalous Hall effect.

[1] S. Grauer *et al.*, Phys. Rev. B **92**, 201304 (2015).

TT 65.9 Thu 12:15 POT 251

Quantum Hall effect in three-dimensional Bi_2Se_3 single crystals — •Olivio Chiatti[1], Marco Busch[1], Sergio Pezzini[2], Steffen Wiedmann[2], Oliver Rader[3], Lada V. Yashina[4], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]High Field Magnet Laboratory, Radboud University Nijmegen, 6525ED Nijmegen, The Netherlands — [3]Helmholtz-Zentrum-Berlin für Materialien und Energie, 12489 Berlin, Germany — [4]Department of Chemistry, Moscow State University, 119991 Moscow, Russia

Topological insulators present surface (or edge) states of helically spin-polarized Dirac fermions, which are readily identified by spectroscopic methods. However, they are not so easily identified in transport, because they can be masked by bulk states. Bi_2Se_3 is one of the prototype topological insulators, but investigating transport by surface states has been hampered by residual bulk charge carriers. We have investigated nominally undoped, high-quality Bi_2Se_3 single crystals, with bulk electron densities of $n \approx 1.8 \cdot 10^{19}$ cm^{-3} and mobilities of up to $\mu \approx 10^3$ cm^2/Vs. Surface states have been confirmed by ARPES measurements [1]. We have measured magnetotransport between $T = 0.3$ K and $T = 72$ K, for tilted magnetic fields up to $B = 33$ T. We observe both Shubnikov-de Haas (SdH) effect and quantum Hall effect (QHE). The SdH oscillations appear dominated by 3D bulk charge carriers. However, the scaling of the QHE with sample thickness can be interpreted as transport over layered 2D states in the bulk.

[1] Chiatti *et al.*, Sci. Rep. **6**, 27483 (2016)

TT 65.10 Thu 12:30 POT 251

The electronic structure of few-quintuple-layer bismuth selenide from first-principles calculations — •Jae Young Kim and Cheol-Hwan Park — Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea

Topological insulators are materials that behave as insulators in the interior, but have conducting surface states protected by time-reversal symmetry [1]. Bi2Se3, a prototypical example of a three-dimensional topological insulator, is a layered material composed of five-atom layers arranged along the z-direction, known as quintuple layers [2]. In this presentation, we will discuss the results of our first-principles calculations on the electronic properties of few-quintuple-layer Bi2Se3 and their relevance to device applications based on topological insulators.

[1] Hasan, M. Z., & Kane, C. L. (2010). Colloquium: topological insulators. Reviews of Modern Physics, 82(4), 3045.

[2] Zhang, H., Liu, C. X., Qi, X. L., Dai, X., Fang, Z., & Zhang, S. C. (2009). Topological insulators in Bi2Se3, Bi2Te3 and Sb2Te3 with a single Dirac cone on the surface. Nature physics, 5(6), 438-442.

TT 66: Graphene: Electronic Properties, Structure and Substrate Interaction I (joint session DY, DS, HL, MA, O, TT, organized by O)

Time: Thursday 10:30–13:00 Location: WIL A317

TT 66.1 Thu 10:30 WIL A317

Charge Puddles in Graphene near the Dirac Point — •Sayanti Samaddar[1,2,3], Indra Yudhistira[4], Shaffique Adam[4,5], Hervè Courtois[2,3], and Clemens Winkelmann[2,3] — [1]II. Physikalisches Institut, RWTH Aachen Otto-Blumenthal-Straße, Turm 28 D-52074 Aachen, Germany — [2]Université Grenoble Alpes, Institut NEEL, F-38042 Grenoble, France — [3]CNRS, Institut NEEL, F-38042 Grenoble, France — [4]Centre for Advanced 2D Materials and Department of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117551, Singapore — [5]Yale-NUS College, 16 College Avenue West, Singapore 138527, Singapore

The charge carrier density in graphene on a dielectric substrate such as SiO2 displays inhomogeneities, the so-called charge puddles. Because of the linear dispersion relation in monolayer graphene, the puddles are predicted to grow near charge neutrality, a markedly distinct property from conventional two-dimensional electron gases. By performing scanning tunneling microscopy/spectroscopy on a mesoscopic graphene device, we directly observe the puddles' growth, both in spatial extent and in amplitude, as the Dirac point is approached. Self-consistent screening theory, together with the consideration of the impact of the STM tip as an electric gate, provides a unified description of both the macroscopic transport properties and the microscopically observed charge disorder.

TT 66.2 Thu 10:45 WIL A317

***Ab-initio* study of the effective Coulomb interactions and Stoner ferromagnetism in hydrogenated graphene** — •Ersoy Sasioglu[1], Hanif Hadipour[2], Christoph Friedrich[3], Stefan Blügel[3], and Ingrid Mertig[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale) Germany — [2]Department of Physics, University of Guilan, 41335 Rasht, Iran — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425Jülich, Germany

Hydrogenation provides a novel way to tune the electronic and optical properties of the graphene. Recent scanning tunneling microscopy experiments have demonstrated that local graphene magnetism can be

selectively switched on and off by hydrogen dimers [1]. Employing *ab-initio* calculations in conjunction with the constrained random-phase approximation [2] we study the strength of the effective Coulomb interaction U in hydrogenated graphene. It is found that the calculated U parameters are smaller than the ones in pristine graphene and depend on the hydrogen concentration. Moreover, the U parameters are very sensitive to the position of hydrogen atoms adsorbed on the graphene lattice. We discuss the instability of the paramagnetic state towards the ferromagnetic one on the basis of calculated U parameters within the Stoner model. Spin-polarized calculations reveal that the experimentally observed itinerant ferromagnetism in hydrogenated graphene can be well described by the Stoner model.

[1] H. González-Herrero *et al.*, Science **352**, 437 (2016).
[2] E. Şaşıoğlu *et al.*, Phys. Rev. B **83**, 121101(R) (2011).

TT 66.3 Thu 11:00 WIL A317

Characterization of CVD-grown graphene on germanium at the atomic scale — •Andreas P. Becker, Wolfang M. Klesse, Mindaugas Lukosius, and Thomas Schroeder — IHP microelectronics GmbH, Frankfurt (Oder), Germany

Graphene is a two-dimensional carbon allotrope where the atoms are arranged in a honeycomb lattice. Especially its extraordinarily high carrier mobility, plasmonic activity and impermeability make it a promising candidate for novel applications in microelectronics, such as high-frequency transistors, sensors and optical modulators.

Direct growth of graphene on silicon is hampered by the formation of covalent bonds. CVD growth of high-quality graphene on transition metal substrates and subsequent transfer of the sheets has proved feasible, however, tenacious metallic contamination obstructs its use in the front-end-of-line of CMOS technology.

As a resort, graphene can be grown on germanium buffer layers, which is one current research focus of the IHP. Specifically, samples grown in the cleanroom are already being routinely investigated by e. g. scanning electron microscopy (SEM) and Raman spectroscopy. But only scanning probe microscopy (SPM) allows to scrutinize graphene layers at the atomic scale and can therefore be an essential complement to such established methods of quality assessment on larger scales.

Accordingly, I will present our latest results on the ex- and in-situ structural characterization of such gr/Ge structures by means of SPM depending on the growth parameters and post-growth annealing procedures.

TT 66.4 Thu 11:15 WIL A317

Observation of photoemission "dark lines" for Ir(111) and graphene/Ir(111) via high-resolution ToF k-microscopy — •Anna Zaporozhchenko-Zymaková[1,2], Dmytro Kutnyakhov[1,3], Katerina Medjanik[1], Christian Tusche[4], Olena Fedchenko[1], Sergey Chernov[1], Martin Ellguth[1], Sergej A. Nepijko[1], Hans-Joachim Elmers[1,2], and Gerd Schönhense[1,2] — [1]Inst. für Physik, Univ. Mainz — [2]MAINZ graduate school — [3]DESY, Hamburg — [4]PGI-6, Forschungszentrum Jülich

ToF k-microscopy [1,2] has been used to analyze emergent photoelectron diffraction effects for UHV/Ir(111) and graphene/Ir(111). We observed a regular pattern of dark lines with circular shape and six-fold symmetry that have been overlooked in previous experiments. Quantitative evaluation along with a model calculation reveals that electrons initially located within the first Brillouin zone can with finite probability be scattered by a reciprocal lattice vector into a state that propagates parallel to the surface. Such electrons vanish due to inelastic scattering events in the vicinity of the surface. This leads to a reduced intensity observed as dark lines. The relevant reciprocal lattice vector corresponds to the lattice of the topmost layer (in our case Ir or graphene). The dark lines appear in a certain photon energy range satisfying the congruence of lattice constant and wavelength. The parallel momentum of the dark lines decreases with increasing photon energy in agreement with the model. The effect has been observed with both p- and s-polarized light at BESSY II (10m NIM). [1] Chernov et al., Ultramic. 159, 453 (2015); [2] Tusche et al., APL 108, 261602 (2016).

TT 66.5 Thu 11:30 WIL A317

Landau Level Spectroscopy of Twisted Graphene Layers on Ir(111) — •Sabina Simon[1], Felix Förschner[1], Vivien Enenkel[1], Fabian Geml[1], Yuriy Dedkov[1], Timo Knispel[2], Charlotte Herbig[2], Thomas Michely[2], and Mikhail Fonin[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Institute of Physics II, University of Köln, 50937 Köln, Germany

Epitaxial growth on metal substrates is known to be one of the most powerful approaches in producing large-scale, high-quality, monolayer graphene. Yet it remains a major challenge to realize the growth of multilayers.

This work is devoted to the investigation of multilayered graphene systems epitaxially grown on a transition metal, namely Ir(111). We address the growth and the structure of large scale twisted graphene bilayers by intercalation of atomic carbon under graphene on Ir(111). We show that the intercalated graphene buffer layer provides sufficient decoupling from the metal substrate, giving a possibility to access the local electronic properties of graphene by means of Landau level spectroscopy. We further discuss the influence of the twist angle on the local electronic properties of the top graphene layer, upon the analysis of the doping level, Fermi velocity of charge carriers, and quasiparticle lifetimes.

TT 66.6 Thu 11:45 WIL A317

Epitaxial growth of graphene via flash annealing of SiC studied by STM, AFM and LEED — •Ismail Baltaci, Malte Schulte, Eugenia Wodopian, Patrick Mehring, and Carsten Westphal — Experimentelle Physik 1, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund

Due to its unique electronic and structural properties graphene is of particular interest for the semi-conductor industry, e.g. as a new material in transistor applications.

In this study we concentrate on an epitaxial growth based on cyclic heating of SiC by direct current, known as flash annealing. In order to yield large and homogeneous graphene layers multiple parameters have to be taken into account such as heating and cooling rates as well as the number of heating cycles.

Determining the number of graphen layers on SiC is achieved by utilizing Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM) and Low Energy Electron Diffraction (LEED). Especially the structural differences between buffer layer and graphen is visualized by STM and LEED measurements. Furthermore, we report on the growth mechanism of graphene.

TT 66.7 Thu 12:00 WIL A317

Surface-assisted self-assembly of graphene nanoribbons — •Axel Enders[1,2], Paulo Costa[2], Jacob Teeter[2], Daniel Miller[3], Eva Zurek[3], and Alexander Sinitskii[2] — [1]Experimentalphysik Va, Universität Bayreuth — [2]University of Nebraska, Lincoln NE 68588, USA — [3]State University of New York at Buffalo, Buffalo 14260, USA

The physical properties of graphene are sensitive to the presence of structural defects, dopants and edges. This creates opportunities to design an electronic bandgap in graphene, which is most consequently exploited in graphene nanoribbons (GNRs), which have edges that are amenable to structural and chemical modification. It is shown that surface-assisted self-assembly is a powerful strategy to build GNRs from the bottom up. As in solution-based self-assembly, also on surfaces the edge structure and chemistry of GNRs is determined by the precursor molecules. But on surfaces the substrate itself can be a control parameter during growth, as can be the method of deposition. Specifically here the self-assembly of 6,11-dibromo-1,2,3,4-tetraphenyltriphenylene and related, appropriately modified precursor molecules was studied on Au(111) and on Cu(111) surfaces. The precursors were deposited under ultrahigh vacuum by two different methods for comparison, which are thermal evaporation and nanoimprinting. Among the significant findings of these studies are the substrate-dependent epitaxial alignment of the ribbons, considerably lower dehalogenation temperatures on Cu(111), and entirely different GNR architectures that can emerge from the same precursors under different conditions.

TT 66.8 Thu 12:15 WIL A317

Lifting Graphene by Alkali Intercalation — •Caio Silva[1], Jiaqi Cai[1], Wouter Jolie[2], Daniela Dombrowski[1,2], Ferdinand Farwick zum Hagen[2], Antonio Martínez-Galera[2], Christoph Schlueter[3], Tien-Lin Lee[3], and Carsten Busse[1,2] — [1]Institut für Materialphysik, Münster, Germany — [2]II. Physikalisches Institut, Köln, Germany — [3]Diamond Light Source Ltd, Didcot, United Kingdom

Intercalation is a versatile tool to tune the properties of graphene grown epitaxially on metal surfaces. Especially alkali metals are efficient to decouple graphene from its substrate and, in addition, induce a strong n-doping on graphene.

In the present work, we used the x-ray standing wave (XSW) te-

chinique to compare the structures resulting from intercalation of a small (Li) and a rather large (Cs) alkali metal between graphene and Ir(111). We noted an opposing behavior during deintercalation: In the case of Cs, different phases $[(\sqrt{3}\times\sqrt{3})R30^\circ_{Ir}, (2\times2)_{gr}]$ coexist, each with a characteristic height of graphene with respect to Ir(111), as revealed by XSW. In the case of Li, however, we find just a single phase of gr/Li/Ir(111) for a wide range of intercalant coverage (1 - 0.2 ML), with a distance between the graphene sheet and the metal surface that is independent on the amount of Li intercalated in between. We explain the contrast between Li and Cs by differences in the delamination energy that has to be paid in order to intercalate the different species.

TT 66.9 Thu 12:30 WIL A317

Giant magneto-photoelectric effect at a graphene edge — •Friedemann Queisser, Ralf Schützhold, Jens Sonntag, Annika Kurzmann, Martin Geller, and Axel Lorke — Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße, Duisburg 47048, Germany

Graphene is a promising material for optical or infrared absorption, as its pseudo-relativistic energy-momentum relation allows for a broad absorption bandwidth. An efficient charge separation can be achieved at a graphene edge in a magnetic field. By solving the Dirac equation, it can be shown that particles and holes move in antipodal directions along the edge [1]. Motivated by the proposed mechanism, an surprisingly high magneto-photocurrent has been measured in suspended graphene [2]. The observed photoresponsitivity (100 incident photons create up to 17 particle-hole pairs) strongly exceeds the predicted value. A possible mechanism to explain the amplification of the magneto-photoeffect relies on the strong Coulomb interaction in graphene: Due to the huge effective fine-structure constant ($\alpha_{\text{graphene}} \gg \alpha_{\text{QED}}$) and the enlarged phase space at the graphene edge, inelastic (Auger-type) scattering amplifies the magneto-photocurrent.

[1] F. Queisser and R. Schützhold *Phys. Rev. Lett.* **111**, 046601 (2013)

[2] J. Sonntag, A. Kurzmann, M. Geller, F. Queisser, A. Lorke, R. Schützhold, arXiv:1505.01762

TT 66.10 Thu 12:45 WIL A317

Magnetism in graphene induced by transition metal and rare earth atomic layers — •Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany

On the Ir(111) surface graphene is physisorbed with a local chemical modulation [1] whose structural and electronic properties can be engineered via atomic intercalation [2,3,4] or molecular adsorption [5,6]. In particular, our *ab initio* density functional theory (DFT) simulations performed for 3*d* transition metal (TM) atoms such as Co [3] and Fe [4] intercalated at the interface between graphene and Ir(111) clearly demonstrated that the graphene layer exhibits a spin-split electronic structure. On the other hand, the strong hybridization between the π electronic states of graphene and the *d* ones of the TM monolayer significantly changes the magnetic properties of the intercalated atoms. Moreover, we investigated if this physical picture remains valid also in the case of the rare earth (RE) atoms with spatially localized magnetic moments such as $4f$ Eu intercalated between graphene and the Ni(111) surface.

This work is supported by DFG through SFB 1238 (Project C01).

[1] C. Busse *et al.*, Phys. Rev. Lett. **107**, 036101 (2011).
[2] W. Jolie *et al.*, Phys. Rev. B **89**, 155435 (2014).
[3] R. Decker *et al.*, Phys. Rev. B **87**, 041403(R) (2013).
[4] R. Decker *et al.*, J. of Phys.: Cond. Matter. **26**, 394004 (2014).
[5] R. Brede *et al.*, Nature Nanotech. **9**, 1018 (2014).
[6] F. Huttmann *et al.*, Phys. Rev. Lett. **115**, 236101 (2015).

TT 67: Topological Insulators II (joint session DS, HL, MA, O, TT, organized by HL)

Time: Thursday 14:45–16:45 Location: POT 251

TT 67.1 Thu 14:45 POT 251

Visualizing the response of Weyl semimetals to Coulomb and magnetic perturbations — •Thomas Bathon[1], Paolo Sessi[1], Yan Sun[2], Florian Glott[1], Zhilin Li[3], Hongxiang Chen[3], Liwei Guo[3], Xialong Chen[3], Markus Schmidt[2], Claudia Felser[2], Binghai Yan[2], and Matthias Bode[1] — [1]Experimentelle Physik II der Universität Würzburg, Würzburg — [2]Max Planck Institute for Chemical Physics of Solids, Dresden — [3]Institute of Physics at the Chinese Academy of Sciences, Peking

Weyl semimetals are a new class of topological materials which led to the emergence of Weyl physics in condensed matter. While photoemission successfully identified Weyl surface states with unique Fermi arcs, their fundamental microscopic properties, such as scattering mechanisms, persistence of spin-coherence, and the reaction to external perturbations, have not been widely investigated so far.
Here, we use TaAs to address these important aspects at the atomic scale by scanning tunneling microscopy and spectroscopy. We deliberately introduce external adatoms to test the response of this class of materials to well-defined Coulomb and magnetic perturbations. We demonstrate that, contrary to topological insulators, they are effectively screened in Weyl semimetals. Our analysis demonstrates that intra- as well as inter-Fermi arc scattering events are strongly suppressed. Additionally, we show that the existence of large parallel segments of spin-split trivial states facing each other makes possible, through scattering, to revert both the propagation direction while simultaneously flipping the spin state, strongly limiting its coherence.

TT 67.2 Thu 15:00 POT 251

Investigation of topological states in proximitized superconducting 2d materials — •Petra Högl, Denis Kochan, Tobias Frank, Martin Gmitra, and Jaroslav Fabian — Insitute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Recently, the appearance of helical edge states in graphene in transition-metal dichalcogenides has been predicted [1]. The presence of these quantum spin Hall states is a precursor for topological insulators. We theoretically investigate such 2d systems proximitized to a s-wave superconductor. As predicted by Fu and Kane [2] the combination of 2d topological insulators and superconductors can lead to the formation of Majorana states. This work has been supported by the Int. Doctorate Program Topological Insulators of the Elite Network of Bavaria, DFG SFB 689, GRK 1570, and by the EU Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

[1] M. Gmitra, D. Kochan, P. Högl, J. Fabian, Phys. Rev. B 93, 155104 (2016)
[2] L. Fu and C. L. Kane, Phys. Rev. B 79, 161408(R) (2009)

TT 67.3 Thu 15:15 POT 251

Tuning Quantum Transport and Interference in Topological Nanowires — •Vincent Sacksteder[1] and Quansheng Wu[2] — [1]W155 Wilson Building, Royal Holloway University of London, Egham Hill, Egham, TW20 0EX, United Kingdom — [2]Theoretical Physics and Station Q Zurich, ETH Zurich, 8093 Zurich, Switzerland

We study the magnetoconductance of topological insulator nanowires in a longitudinal magnetic field, including Aharonov-Bohm, Altshuler-Aronov-Spivak, perfectly conducting channel, and universal conductance fluctuation effects. We show that changing the Fermi energy can tune a wire from from ballistic to diffusive conduction and to localization. In both ballistic and diffusive single wires we find both Aharonov-Bohm and Altshuler-Aronov-Spivak oscillations with similar strengths, accompanied by quite strong universal conductance fluctuations (UCFs), all with amplitudes between 0.3 and 1 conductance quanta. This contrasts strongly with the average behavior of many wires, which shows Aharonov-Bohm oscillations in the ballistic regime and Altshuler-Aronov-Spivak oscillations in the diffusive regime, with both oscillations substantially larger than the conductance fluctuations. We also show that in long wires the perfectly conducting channel is visible at a wide range of energies within the bulk gap. We present typical conductance profiles at several wire lengths, showing that conductance fluctuations can dominate the average signal. Similar behavior will be found in carbon nanotubes.

Coffee Break

TT 67.4 Thu 16:00 POT 251

time-reversal-breaking topological phases in anti-ferromagnetic Sr_2FeOsO_6 films — •Xiao-Yu Dong[1,2], Sudipta Kanungo[3,4], Binghai Yan[2,3], and Chao-Xing Liu[5] — [1]Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, Beijing 100084, P.R.China — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187, Dresden, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [4]Center for Emergent Matter Science (CEMS), RIKEN, 2-1, Hirosawa, Wako, Saitama 351-0198, Japan — [5]Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802-6300, USA

In this work, we studied time-reversal-breaking topological phases as a result of the interplay between anti-ferromagnetism and inverted band structures in anti-ferromagnetic double perovskite transition metal Sr_2FeOsO_6 films. By combining the first principles calculations and analytical models, we demonstrate that the quantum anomalous Hall phase and chiral topological superconducting phase can be realized in this system. We find that to achieve time-reversal-breaking topological phases in anti-ferromagnetic materials, it is essential to break the combined symmetry of time reversal and inversion, which generally exists in anti-ferromagnetic structures. As a result, we can utilize an external electric gate voltage to induce the phase transition between topological phases and trivial phases, thus providing an electrically controllable topological platform for the future transport experiments.

TT 67.5 Thu 16:15 POT 251

Surface state-dominated photoconduction and THz-generation in topological Bi_2Te_2Se-nanowires — •Marinus Kundinger[1], Paul Seifert[1], Kristina Vaklinova[2], Klaus Kern[2,3], Marko Burghard[2], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physics-Department, Technical University of Munich, Am Coulombwall 4a, D-85748 Garching, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [3]Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Topological insulators constitute a fascinating class of quantum materials with non-trivial, gapless states on the surface and trivial, insulating bulk states. In revealing the optoelectronic dynamics in the whole range from femto- to microseconds, we demonstrate that the long surface lifetime of Bi_2Te_2Se-nanowires allows to access the surface states by a pulsed photoconduction scheme and that there is a prevailing bolometric response of the surface states. The interplay of the surface state dynamics on the different timescales gives rise to a surprising physical property of Bi_2Te_2Se-nanowires: their pulsed photoconductance changes polarity as a function of laser power. Moreover, we show that single Bi_2Te_2Se-nanowires can be used as THz-generators for on-chip high-frequency circuits at room temperature. Our results open the avenue for single Bi_2Te_2Se-nanowires as active modules in optoelectronic high-frequency and THz-circuits.

We acknowledge financial support by the DFG priority program SPP 1666 'topological insulators'.

TT 67.6 Thu 16:30 POT 251

THz radiation induced helicity sensitive photocurrents in type-II GaSb/InAs quantum well structures — •Helene Plank[1], Johanna Pernul[1], Tanja Hummel[1], Georg Knebl[2], Pierre Pfeffer[2], Martin Kamp[2], Susanne Mueller[3], Thomas Tschirky[3], Sergey A. Tarasenko[4], Werner Wegscheider[3], Sven Höfling[2,5], and Sergey D. Ganichev[1] — [1]Terahertz Center, University of Regensburg, Regensburg, Germany — [2]Technische Physik University of Würzburg, Würzburg, Germany — [3]ETH Zurich, Solid State Physics Laboratory, Zurich, Switzerland — [4]Ioffe Institute, St.Petersburg, Russia — [5]University of St. Andrews, St. Andrews, United Kingdom

We report on the observation of terahertz radiation induced helicity sensitive photocurrents in GaSb/InAs quantum wells in the inverted regime. The photocurrent reverses its direction upon switching the circular polarization from left- to right-handed. The origin of the photocurrent depends on the experimental geometry and the Fermi energy position. For illuminating the sample centre, it stems from asymmetric scattering of free carriers excited by electric THz field [1]. At normal incidence or for Fermi energies in the gap it vanishes. The situation changes at the sample edges, where is it observed for both cases. We show that this edge current is caused by optical excitation of helical edge states in 2D topological insulators. The observed sign inversion upon changing the photon helicity is attributed to selection rules of optical transitions. We discuss the photocurrent behaviour and present microscopic models. [1] H. Plank *et al.*, Physica E **85**, 193 (2017).

TT 68: SYLM: Optics and Light-Matter Interaction with Excitons in 2D Materials (joint symposium DS, DY, HL, TT, organized by HL)

Time: Thursday 15:00–18:30 Location: HSZ 02

Invited Talk TT 68.1 Thu 15:00 HSZ 02

Light matter interaction in TMDs and their heterostructures — •Ursula Wurstbauer — Walter Schottky Institute and Physics-Department, TU Munich — Nanosystems Initiative Munich (NIM)

Transition metal dichalcogenides (TMDs) such as MoS2 are of current interest for optoelectronic, sensing and energy harvesting applications, but also for studying fundamental aspects of light-matter interaction in strictly two-dimensional semiconductors [1,2]. These materials exhibit a high sun light absorbance of up to 15% in the monolayer limit [3], photocatalytic stability [4] and access to excitonic phenomena in van der Waals heterostructures. We access the complex dielectric function and their fine-structure by spectroscopic imaging ellipsometry [3]. The importance of excitonic effects emerge also in resonant Raman spectroscopy, where unexpected polarization dependence points towards strong exciton-phonon coupling in MoS2. We furthermore achieve strong signatures for interlayer coupling and the formation of presumably long-lived interlayer excitons in such van der Waals heterostructures.

We acknowledge support by BaCaTeC and DFG via Nanosystems Initiative Munich (NIM), and project WU 637/4-1.

[1] U. Wurstbauer et al. arXiv:1611.05255 (2016). [2] B. Miller, et al., Appl. Phys. Lett. 106, 122103 (2015). [3] S. Funke et al., J. Phys. Condens. Matter 28, 385301 (2016). [4] E. Parzinger et al. ACS Nano 9(11), 11302 (2015).

Invited Talk TT 68.2 Thu 15:30 HSZ 02

Quantum optics with deterministically positioned quantum emitters in a two-dimensional semiconductor — •Brian Gerardot — Institute of Photonics and Quantum Sciences, SUPA, Heriot-Watt University, Edinburgh EH14 4AS, UK

The emergence of single quantum emitters in layered transition metal dichalcogenide semiconductors offers new opportunities to construct a scalable quantum architecture with a coherent light-matter interface. Here I will present results taking steps in this direction. First, using nanoscale strain engineering, we deterministically achieve a two-dimensional lattice of quantum emitters in an atomically thin semiconductor. We create point-like strain perturbations in mono-and bi-layer WSe2 which locally modify the band-gap, leading to efficient funnelling of excitons towards isolated strain-tuned quantum emitters that exhibit high-purity single photon emission. Next, we perform resonance fluorescence and high-resolution photoluminescence excitation spectroscopy of these isolated, localized 2D excitons to reveal near ideal single photon fluorescence and uncover dark exciton states ~ 5meV blue-shifted from the bright exciton states. The high-purity single photon emission is stable and bright, yielding detected count rates up to 3 MHz. These results yield a route for intriguing investigations of the spin and valley coherence of localized excitons in 2D-transition metal dichalcogenide semiconductors.

Invited Talk TT 68.3 Thu 16:00 HSZ 02

Light-matter coupling with atomic monolayers in microcavities — •Christian Schneider — Technische Physik, University of Wuerzburg, Germany

Transition metal dichalcogenides represent a novel emerging class of materials which seems almost ideal to study light-matter coupling in solid state. In this talk, I address the case of a single atomic monolayer

embedded in dielectric and metal-based photonic structures. I will discuss the formation of exciton-polaritons from cryogenic temperatures up to ambient conditions in compact and flexible Tamm-structures. I will also discuss peculiarities which arrise from the moderate quality factors in these structures, yielding significantly different anticrossings in luminescence and reflection. Finally, a focus is set on the interplay of excitons and trions, both in the weak and strong coupling limit.

Coffee Break

Invited Talk TT 68.4 Thu 17:00 HSZ 02
Properties of Synthetic 2D Materials and Heterostructures — •Joshua Robinson — Pennsylvania State University, University Park, PA, USA

The last decade has seen nearly exponential growth in the science and technology of two-dimensional materials. Beyond graphene, there is a huge variety of layered materials that range in properties from insulating to superconducting. Furthermore, heterogeneous stacking of 2D materials also allows for additional dimensionality for band structure engineering. In this talk, I will discuss recent breakthroughs in two-dimensional atomic layer synthesis and properties, including novel 2D heterostructures and novel 2D nitrides. Our recent works include development of an understanding of substrate impact on 2D layer growth and how we can tune the substrate to acheive near-single crystal 2D materials over large areas. I will also dsicuss doping of 2D materials with magentic elements, selective area synthesis of 2D materials, and the first demonstration of 2D gallium nitride (2D-GaN). Our work and the work of our collaborators has lead to a better understanding of how substrate not only impacts 2D crystal quality, but also doping efficiency in 2D materials, and stabalization of nitrides at their quantum limit.

Invited Talk TT 68.5 Thu 17:30 HSZ 02
Exciton spectroscopy in transition metal dichalcogenide monolayers and van der Waals heterostructures — •Bernhard Urbaszek — CNRS - Toulouse University, France

Excitons in transition metal dichalcogenide monolayers (MLs) provide exciting opportunities for applications and new frontiers in physics: (i) with binding energies of several hundred meV, excitons dominate optical properties even at room temperature, (ii) strong exciton oscillator strength leads to absorption of up to 20 % per ML, and (iii) the interband selection rules are valley selective. In combination with strong spin-orbit splittings this allows studying spin-valley physics. Although ML samples on Si/SiO2 substrates are widely studied in the literature, conclusive measurements on the excited exciton states and fine structure (2s/2p) are still missing. In hBN / ML WSe2 / hBN samples we measure for the linewidth of the neutral and charged exciton emission values down to 1.6 meV at T=4K, close to the homogenous limit. This allows us to perform 1 and 2-photon spectroscopy which reveal details previously masked by inhomogeneous broadening. Also, we demonstrate control of the exciton valley coherence in ML WSe2 on SiO2 by tuning the applied magnetic field B perpendicular to the ML plane. Linearly polarized laser excitation prepares a coherent superposition of valley states and the induced valley Zeeman splitting between K+ and K- results in a change of the oscillation frequency of the superposition of valley states. This corresponds to a rotation of the exciton valley pseudo-spin by angles as large as 30 degrees for fields up to B=9T.

Invited Talk TT 68.6 Thu 18:00 HSZ 02
Strain-induced single-photon emitters in layered semiconductors — •Rudolf Bratschitsch — Westfälische Wilhelms-Universität Münster, Münster, Deutschland

Single-photon sources are important building blocks for quantum information technology. Emitters based on solid-state systems provide a viable route for their integration in photonic devices. Recently, we have found single-photon emitters in the atomically thin semiconductor WSe2 [1]. We show that the quantum light sources are strain-induced and demonstrate deterministic positioning of the emitters on the nanoscale [2]. Finally, we present single-photon emission from the layered semiconductor GaSe and provide evidence that the incorporated non-classical light sources are also strain-induced [3].

[1] P. Tonndorf et al., Optica 2, 347 (2015)
[2] J. Kern et al., Advanced Materials 28, 7101 (2016)
[3] P. Tonndorf et al., 2D Materials (2016)

TT 69: Focus Session: Superconductivity in the Vicinity of a Quantum Critical Point

Unconventional (i.e., nonphonon-mediated) superconductivity is often observed at the border of magnetic order. The suppression of the long-range order opens up a wide parameter regime where the physics may be controlled by an underlying quantum critical point (QCP). Presently, a central question in condensed matter concerns the interplay between quantum criticality and unconventional superconductivity in these strongly correlated electron systems. This session covers the central advances, reported in the last years, connecting quantum criticality and superconductivity in the major classes of unconventional superconductors.

Organization: Cornelius Krellner, Universität Frankfurt; Philipp Gegenwart, Universität Augsburg; Roser Valentí, Universität Frankfurt

Time: Thursday 15:00–18:15 Location: HSZ 03

Invited Talk TT 69.1 Thu 15:00 HSZ 03
The Antiferromagnet $YbRh_2Si_2$ - a New Heavy-Fermion Superconductor — •Frank Steglich — MPI CPfS Dresden, Germany — CCM, ZJU Hangzhou, China — IOP, CAS, Beijing, China

While unconventional superconductivity (SC) often occurs in the vicinity of quantum critical points (QCPs) in antiferromagnetic (AF) heavy-fermion metals, no SC has so far been observed near the QCP induced by a small magnetic field in $YbRh_2Si_2$. Here, we explore results of magnetic and calorimetric measurements on $YbRh_2Si_2$ down to $T = 1$ mK (E. Schuberth *et al.*, Science **351**, 485 (2016)). They reveal the onset of a hybrid nuclear-electronic type of AF order dominated by the Yb-derived nuclear spins at T_A slightly above 2 mK and the subsequent development of SC at $T_c = 2$ mK. The initial slope of the upper critical field curve, $B_{c2}(T)$, at T_c is found to be as large as $-B'_{c2} \simeq 25$ T/K. This indicates that the effective charge-carrier mass must be of the order of several 100 m_{el}, implying that the superconducting state is associated with the Yb-derived $4f$-electronic rather than nuclear spins. Therefore, the theoretical possibility of superheavy-fermion SC based upon an underlying nuclear Kondo effect can be ruled out. In conclusion, we ascribe the formation of Cooper pairs in $YbRh_2Si_2$ to the critical fluctuations associated with the unconventional, Mott-type, QCP of this antiferromagnet, which are revealed when the primary electronic order is diminished by the competing nuclear-dominated hybrid order. Our results demonstrate a new means to reach a field-induced QCP and provide further evidence that SC in the vicinity of AF QCPs is a general phenomenon.

Invited Talk TT 69.2 Thu 15:30 HSZ 03
Quantum Criticality in Cuprate and Iron Based Superconductors — •Antony Carrington — University of Bristol, U.K.

I will review experiments which show that $BaFe_2(As_{1-x}P_x)_2$ is perhaps the best example of a quantum critical superconductor with a high T_c. Quantum oscillation cyclotron mass, specific heat and magnetic penetration depth are all strongly enhanced over a narrow range of x. Interestingly this increase in mass does not influence either the lower or upper critical fields in the expected way.

I will also discuss the applicability of quantum criticality to the cuprates. By measuring quantum oscillations in $YBa_2Cu_4O_8$ under hydrostatic pressure we are able to show that the quasiparticle mass *decreases* as maximum T_c is approached. This result is opposite to the

behaviour found when $YBa_2Cu_3O_{7-\delta}$ is tuned towards maximum T_c by oxygen doping. Our results suggest that the proximity of the CDW end point to the maximum in T_c with doping is coincidental and that therefore quantum fluctuations of the CDW order do not boost T_c in the cuprates.

Invited Talk TT 69.3 Thu 16:00 HSZ 03

Evolution of the Fermi Surface of the Nematic Superconductors $FeSe_{1-x}S_x$ — •Amalia Coldea — University of Oxford

I will present the evolution of the Fermi surfaces and electronic interactions across the nematic phase transition in single crystals of $FeSe_{1-x}S_x$ using Shubnikov-de Haas oscillations in high magnetic fields up to 45 tesla in the low temperature regime. The unusually small and strongly elongated Fermi surface of FeSe increases monotonically with chemical pressure, x, due to the suppression of the in-plane anisotropy except for the smallest orbit which suffers a Lifshitz-like transition once nematicity disappears. Even outside the nematic phase the Fermi surface continues to increase, in stark contrast to the reconstructed Fermi surface detected in FeSe under applied external pressure. I will present the unusual signatures of orbital-dependent quasiparticle mass renomalization suppressed for those orbits with dominant $d_{xz/yz}$ character, but unusually enhanced for those orbits with dominant dxy character. The lack of enhanced superconductivity outside the nematic phase in $FeSe_{1-x}S_x$ suggest that nematicity may not play the essential role in enhancing Tc in these systems.

15 min. break.

Invited Talk TT 69.4 Thu 16:45 HSZ 03

Superconductivity near Structural Instabilities — •Malte Grosche — Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK

Complex materials frequently display an interesting interplay between structural and electronic instabilities, which can often be studied effectively under applied pressure. This talk will present some recent examples, including (i) a structural quantum critical point and its consequences for superconductivity in the quasi-skutterudite system $(Sr/Ca)_3(Ir/Rh)_4Sn_{13}$ [1], (ii) unconventional superconductivity in YFe_2Ge_2 and its connection with superconductivity in the high-pressure collapsed tetragonal phase of alkaline-metal iron arsenides [2], and (iii) strong-coupling superconductivity in the incommensurate high-pressure host-guest structure of elemental bismuth.

[1] Goh et al., Phys. Rev. Lett. **114,** 097002 (2015)
[2] Chen et al., Phys. Rev. Lett. **116,** 127001 (2016)

Invited Talk TT 69.5 Thu 17:15 HSZ 03

An Empirical Approach to the 2 mK Transition in $YbRh_2Si_2$ — •Christoph Geibel, Manuel Brando, and Alexander Steppke — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The Kondo lattice system $YbRh_2Si_2$ is located extremely close to a quantum critical point (QCP) separating the magnetic ordered from the paramagnetic ground state. This results in a number of very unusual properties whose origins are controversially discussed. Recently an abrupt drop in the magnetic susceptibility at 2 mK provided evidence for a combined nuclear-electronic magnetic and superconducting transition [1]. However, the scenario proposed in [1], being based on a Landau model with a large number of free parameters, met some skepticism. Here we analyze the specific properties of $YbRh_2Si_2$ in view of possible mechanisms for this 2 mK transition. After introducing how hyperfine interaction works for Yb, we single out some very peculiar properties of $YbRh_2Si_2$ which result in a specific and unique situation for the interplay between 4f and nuclear moments. Below a few mK the AFM state formed at 70 mK, because of its tiny ordered 4f moment, becomes inherently unstable against the formation of a state with a larger ordered moment. Our analysis strongly supports the existence of a combined nuclear-electronic transition in the mK range in $YbRh_2Si_2$, but indicates that the ordered 4f moment should increase at this transition, in contrast to the decrease proposed in [1].

[1] E. Schuberth et al., Science 351, 485 (2016)

TT 69.6 Thu 17:45 HSZ 03

THz response of $CeCoIn_5$ and evolution of effective mass in the non-Fermi liquid regime — Uwe S. Pracht[1], Martin Dressel[1], Jernej Mravlje[2], Peter Wölfle[3], Ryota Endo[4], Tatsuya Watashige[4], Yousuke Hanaoka[4], Masaaki Shimozawa[5], Takahito Terashima[4], Takasada Shibauchi[5], Yuji Matsuda[4], and •Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Jozef Stefan Institute, Ljubljana, Slovenia — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany — [4]Kyoto University, Kyoto, Japan — [5]University of Tokyo, Chiba, Japan

$CeCoIn_5$ is a heavy-fermion superconductor that exhibits non-Fermi-liquid properties in the metallic state below 30 K that are interpreted in terms of quantum criticality. The strong evolution of the quasiparticle effective mass with temperature or energy, which is characteristic for heavy fermions, takes place in this normal-state regime, but is typically difficult to access experimentally. Optical spectroscopy on metals can reveal the temperature- and frequency-dependent effective mass and transport scattering rate in and beyond the quantum-critical regime.

Here we perform THz spectroscopy on $CeCoIn_5$ thin films in wide temperature (3 K to 150 K) and frequency (0.2 THz to 1.1 THz) regions that match in energy [1], and we employ an extended Drude analysis. We find strong frequency and temperature dependence of the scattering rate and the effective mass, and we discuss the implications for understanding the evolution of the heavy-fermion, non-Fermi-liquid state of $CeCoIn_5$.

[1] U.S. Pracht *et al.*, J. Magn. Magn. Mater. **400**, 31 (2016).

TT 69.7 Thu 18:00 HSZ 03

Approaching a Van Hove Singularity in Sr_2RuO_4 Using Uniaxial Stress — •Mark E. Barber[1,2], Alexandra S. Gibbs[1,3], Yoshiteru Maeno[4], Clifford W. Hicks[2], and Andrew P. Mackenzie[1,2] — [1]Scottish Universities Physics Alliance (SUPA), School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, Dresden 01187, Germany — [3]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot OX11 OQX, United Kingdom — [4]Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan

Sr_2RuO_4 is an unconventional superconductor with a well characterised Fermi liquid normal state. It is known that one of its three conduction bands lies in close proximity to a Van Hove singularity and we show that by the application of uniaxial pressure the Fermi level can be made to traverse the Van Hove singularity. For the first time we can tune through this topological Liftshitz transition using a clean and continuous tuning parameter. We observe more than a factor of 2.3 enhancement of T_c and quantum critical behaviour in the normal state properties.

TT 70: Superconductivity: Fe-based Superconductors - Theory

Time: Thursday 15:00–18:15 Location: HSZ 103

Invited Talk TT 70.1 Thu 15:00 HSZ 103

New Developments in the Theory of STM on Unconventional Superconductors — •Andreas Kreisel — Institut für Theoretische Physik, Uni Leipzig, Germany — Niels Bohr Institute, Copenhagen, Denmark

Scanning Tunneling Microscopy (STM) has become a widely used experimental technique to study superconductivity, yet new approaches are unraveling so far unknown properties. A number theories have been used to explain the qualitative origin of superconducting pairing in Fe-based superconductors (FeSC), but quantitative, material-specific comparisons to experimental results have been made in few cases only. Here, a novel approach to theoretical simulation of STM is outlined which combines first-principles calculations to obtain material-specific Wannier functions and lattice Green functions from BdG or T-matrix calculations. The method takes into account crystal symmetries such that it improves the traditional lattice calculations from two perspectives: Effects of the tunneling layers are contained qualitatively and the spatial resolution is not limited to the lattice spacing, thus comparable to the resolution of experimentally available data. By calculating the local density of states relevant for the tunneling process, it is possible to simulate images of impurities on the surface of superconductors. As examples, we study disorder in a cuprate superconductor and a FeSC and discuss conclusions that can be drawn about the order parameter when comparing to experimental observations.

TT 70.2 Thu 15:30 HSZ 103

Tilting the balance towards d-wave in iron-based superconductors — Mario Fink and •Ronny Thomale — Institut für Theoretische Physik, Universität Würzburg, 97074 Würzburg, Germany

The interplay of interactions and Fermi surface topology in iron-based superconductors can promote s-wave and d-wave superconductivity as competitive canditates. From the theoretical limit of zero temperature, we develop a phenomenological thermodynamic argument how a weak perturbation such as small but finite temperature or an applied Zeeman field H_z can favor a nodal d-wave state over a nodeless s-wave state. This preference occurs as the quasiparticles in the nodal regime gain energy by polarization with respect to the applied field, or generate entropy at small finite temperature. We speculate that $K_xBa_{1-x}Fe_2As_2$ for large hole doping could be a viable scenario for such a magnetically or entropically induced transition from s-wave to d-wave superconductivity.

TT 70.3 Thu 15:45 HSZ 103

Competition of SDW and iCDW and the role of spin-orbit coupling — •Felix Ahn[1], Fabian Lambert[1], Maria N. Gastiasoro[2], Daniel D. Scherer[2], Brian M. Anderson[2], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark

The magnetic stripe phase is a mutual feature of most the iron-based superconductors and can be described in the basis of the iron $3d$-orbitals or, alternatively, it can be described within the band basis where magnetism occurs as a Fermi surface instability. In this work, we show how spin-orbit coupling causes an intrinsic spin-space anisotropy that is necessarily relevant for the different magnetic phases and that it lifts the Dirac cones of the nodal spin density-wave (SDW) order parameter, in particular. Most importantly, we show that spin-orbit coupling adds an inevitable companion to the SDW phase, namely a charge-current density-wave that is often dubbed imaginary charge density-wave (iCDW).

TT 70.4 Thu 16:00 HSZ 103

s+is Superconductivity with incipient bands: doping dependence and STM signatures — •Jakob Böker, Pavel Volkov, and Ilya Eremin — Institut fur Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Motivated by the recent observations of small Fermi energies and comparatively large superconducting gaps, present on bands located below the Fermi energy(incipient bands) in iron-based superconductors, we analyse the doping evolution of superconductivity in a four-band model in the BCS-BEC crossover regime for the iron pnictides. Similar to the BCS case we find that with hole doping the phase difference between superconducting order parameters of the hole bands changes from 0 to π through an intermediate $s+is$ state breaking time-reversal symmetry. However, in the BCS-BEC crossover phase this transition occurs in the region where electron bands are already above the Fermi level and that the chemical potential renormalization leads to significant broadening of the $s+is$ region. This makes the observation of this phase easier in experiment. We further present the qualitative features of the $s+is$ state that can be observed in scanning tunnelling microscopy (STM) experiments.

TT 70.5 Thu 16:15 HSZ 103

Inelastic STM in LiFeAs — •Patrik Hlobil, Jörg Schmalian, Wulf Wulfhekel, and Jasmin Jandke — KIT

Scanning tunneling microscopy (STM) has been shown to be a powerfulexperimental probe to detect electronic excitations and further allows to deduce fingerprints of bosonic collective modes in superconductors. Here, we demonstrate that the inclusion of inelastic tunnel events is crucial for the interpretation of tunneling spectra of unconventional superconductors and allows to directly probe electronic and bosonic excitations via STM. We apply the formalism to the iron based superconductor LiFeAs. With the inclusion of inelastic contributions, we find strong evidence for a non-conventional pairing mechanism, likely via magnetic excitations.

15 min. break.

TT 70.6 Thu 16:45 HSZ 103

Superconducting fluctuations with small Fermi energies: the case of FeSe — •Pavel A. Volkov, Ilya Eremin, and Konstantin B. Efetov — Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Recent experiments imply the presence of strong superconducting fluctuations above T_c in FeSe. It has been suggested that the observed effects could be due to the presence of a band with an anomalously small Fermi energy $\varepsilon_F \sim \Delta$. We report theoretical analysis of superconducting fluctuations in a two-band model with one of the bands having small ε_F. While close to T_c the system is described by a conventional Ginzburg-Landau theory (unless an accidental degeneracy between superconducting channels is present), the microscopic expressions for the coefficients differ from the ones obtained in the usual BCS ($\varepsilon_F \gg \Delta$) theory. We also present analytical expressions for fluctuation effects valid at elevated temperatures. On the basis of our results, we discuss the possible relevance of the BCS-BEC crossover to the phenomena observed in FeSe.

TT 70.7 Thu 17:00 HSZ 103

Interfacial electron-phonon coupling strength and high-T_c superconductivity in monolayer FeSe/$SrTiO_3$ — •Alex Aperis and Peter M. Oppeneer — Uppsala University, Sweden

Superconductivity in monolayer FeSe on $SrTiO_3$ reaches mysteriously high transition temperatures of typically 50-70 K and up to 100 K, much higher than the T_c=8 K of bulk FeSe. At the FeSe/$SrTiO_3$ interface, a coupling between $SrTiO_3$ phonons and FeSe electrons that manifests as electron replica bands, is commonly believed to enhance T_c moderately but not enough to fully explain it. Here, we employ fully anisotropic, full bandwidth multiband Eliashberg calculations to examine the impact of these phonons on the superconducting state of FeSe/$SrTiO_3$. We find that the interfacial electron-phonon interaction which is hidden behind the seemingly weak coupling constant, λ_m=0.4, fully accounts for the high-T_c while also solving puzzling experimental facts like the s-wave symmetry and replica bands. Our calculations indicate that replica band formation has a T_c-decreasing effect which is nevertheless overcompensated by T_c-enhancing Cooper pairing at bands away from the Fermi level. We predict this mechanism to produce a strong coupling dip-hump signature in the tunnelling spectra.

TT 70.8 Thu 17:15 HSZ 103

Orbitally resolved superconductivity within FLEX: doping evolution of the FeSe monolayer — •Andreas Linscheid[1], Yan Wang[2], Saurabh Maiti[1], Steven Johnston[2], and Peter Hirschfeld[1] — [1]Department of Physics, University of Florida,

Gainesville — [2]Department of Physics and Astronomy, University of Tennessee

FeSe-derived materials have been studied by several recent experiments concerning a number of phenomena that still lack a concise explanation. First, the nature of the pairing in materials with only electron pockets at the Fermi level is still under debate, with proposed explanations by both electronic s++ and s+- and/or phononic pairing. Second, the effective quasi particle mass at the Fermi level is very orbital dependent which likely affects the pairing and may require to solve the superconducting (SC) pairing in the space of orbitals. The effective mass is bound to have consequences for the spin- and charge fluctuations and the problem should therefore be solved self-consistently. In this work, we extend our previous study [PRL 117, 077003] and describe the electron doped FeSe in an orbitally resolved microscopic model. Starting from the normal state DFT band structure, we apply orbitally resolved FLEX to study the system in the SC state, as well as in the magnetic phase. By retaining full momentum resolution, we can also include strong forward scattering by phonons in the FeSe/STO system and discuss the self-consistent influence of the orbitally-resolved quasi particle mass on SC as a function of doping.

TT 70.9 Thu 17:30 HSZ 103

Enhancement of superconductivity by interfacial phonons in perovskite-clad FeAs monolayers — Seokhwan Choi[1], Won-Jun Jang[1], Hyun-Jung Lee[2], Jong Mok Ok[2], Hyun Woo Choi[1], Alex Taekyung Lee[3], •Alireza Akbari[2,4], Ken Nakatsukasa[5], Yannis K. Semertzidis[6], Yunkyu Bang[7], Steven Johnston[5], Jun Sung Kim[2], and Jhinhwan Lee[1] — [1]Korea Advanced Institute of Science and Technology, Daejeon, Korea — [2]Asia Pacific Center for Theoretical Physics, Pohang, Korea — [3]Columbia University, New York 10027, USA — [4]Pohang University of Science and Technology, Pohang, Korea — [5]University of Tennessee, Knoxville, Tennessee, USA — [6]Institute of Basic Science, Daejeon, Korea — [7]Chonnam National University, Kwangju, Korea

The physics at interfaces between monolayer iron-based superconductors (FeSC) and perovskite substrates has received considerable attention due to the unusually high T_c of 100 K found recently in monolayer FeSe on $SrTiO_3$. We present a quasiparticle interference (QPI) study which provides a strongest-ever proof of enhancement of the Fe-based superconductivity (FeSC) by the forward-scattering interfacial phonons in the system of the perovskite-clad FeSC monolayers. Furthermore, the self-assembled heterostructure studied here shows stronger electron-phonon coupling consistent with the doubled interfaces per FeSC monolayer and has greater applicability due to its massively parallel superconducting layers compared with the monolayer counterpart.

[1] S. Choi et al., arXiv:1608.00886.

TT 70.10 Thu 17:45 HSZ 103

Structural Properties and Magnetic Behavior of the New Iron-based Superconductor $CaKFe_4As_4$ — •Felix Lochner[1,2], Ilya Eremin[2], and Tilmann Hickel[1] — [1]Computergestütztes Materialdesign, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany

The iron-based superconductor $CaKFe_4As_4$ is one of the most famous representative of the new 1144 family of the iron pnictides. Because of the combination of alcali and alcaline-earth metals $CaKFe_4As_4$ is hole-doped itself and reaches a transition temperature of $T_c = 35$ K [1]. We calculate *ab initio* the electronic structure and internal parameters by using density functional theory for several magnetic configurations. In contrast to other iron-based superconductors we find that the d_{xy}-orbital contributes not much to the Fermi-surface, whereas the $d_{x^2-y^2}$- and d_{z^2}-orbitals are showing a strong contribution. This behavior is related to the shift of the FeAs-layer away from its high-symmetry position [2]. Hereby we focus on the orbital-resolved electronic bandstructure to estimate the strength of the electronic interactions.

[1] W. R. Meier *et. al.*, PRB **94**, 064501 (2016)
[2] D. Mou *et. al.*, arXiv:1606.05643

TT 70.11 Thu 18:00 HSZ 103

Chromium analogues of iron-based supercondictors — •Martin Edelmann[1], Giorgio Sangiovanni[1], Massimo Capone[2], and Luca de' Medici[3] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136 Trieste, Italy — [3]European Synchrotron Radiation Facility, 71 Av. des Martyrs, Grenoble, France

The present talk encompasses the results of our studies of $BaCr_2As_2$, the Cr equivalent of the 122 iron-based superconductor (FeSC) $BaFe_2As_2$. In the respective compound, Cr nominally hosts 4 electrons in its d orbitals, whereas Fe hosts six, placing Cr on the other side of half-filling. Therefore, one expects behaviour of the Cr compound that is specular to $BaFe_2As_2$. We conducted DFT+DMFT studies on the PM and G-type AFM phase as well as slave-spin mean field (SSMF) calculations on the PM phase [1]. We show that dynamical correlations are necessary to narrow the discrepancy between the Sommerfeld coefficient as accessed by theoretical studies and the experimental value. Through SSMF one finds that the $BaCr_2As_2$ mirrors the $BaFe_2As_2$ compressibility, where the $BaCr_2As_2$ compound phase diagram displays a crossover from a weakly to a strongly correlated metal. We infer that, similar to $BaFe_2As_2$, $BaCr_2As_2$ can be pushed into the SC regime with the proper amount of electron doping and/or negative pressure, introducing a new, interesting family of SCs.

[1] M. Edelmann, G. Sangiovanni, M. Capone, L. de' Medici, arXiv:1610.10054

TT 71: Superconductivity: Cryodetectors and Cryotechnique

Time: Thursday 15:00–18:00 Location: HSZ 201

TT 71.1 Thu 15:00 HSZ 201

Photon number resolving superconducting nanowire single-photon detectors — •Ekkehart Schmidt[1], Eric Reutter[1,2], Hannes Rotzinger[2], Konstantin Ilin[1], Alexey V. Ustinov[2], and Michael Siegel[1] — [1]Institut für Mikro- und Nanoelektronische Systeme (IMS), Karlsruher Institut für Technologie, Herzstraße 16, 76187 Karlsruhe, Deutschland — [2]Physikalisches Institut (PHI), Karlsruher Institut für Technologie, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Deutschland

Superconducting nanowire single-photon detectors (SNSPDs) are attractive for a variety of applications like integrated photonics, quantum key distribution and deep space communication. They have a high detection efficiency, single photon sensitivity, low dark count rate and very good time resolution but they lack intrinsic photon number resolution (PNR). By splitting of the SNSPD in several pixels using integrated shunts [1] quasi-PNR can be achieved, thereby allowing amplitude multiplexing of detected number of photons. We developed technology and demonstrated quasi-PNR functionality of SNSPDs made of 4.9 nm thick and 80 nm wide NbN nanowires on sapphire, which were shunted by integrated palladium resistors with a resistance of ~20 Ohms. Optical excitation of these detectors with an SWIR fs-laser clearly shows a power-depending photon statistic. Further details on the study of operation and optical response of quasi-PNR SNSPD will be presented and discussed.

[1]S. Jahanmirinejad et al. Opt. Express 20 2012, 5017-5028

TT 71.2 Thu 15:15 HSZ 201

Current Sensing Noise Thermometer for Milli-Kelvin Temperatures with optimized dc-SQUIDs for Cross Correlated Readout — •Felix Mücke, Andreas Reifenberger, Marius Hempel, Daniel Richter, Sebastian Kempf, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, INF 227, Universität Heidelberg, 69120 Heidelberg

Within our search for easy-to-use reliable thermometers for milli-Kelvin and micro-Kelvin temperatures we recently developed a noise thermometer, where the Johnson current noise of a massive cylinder of high purity silver is monitored simultaniously by two current sensing dc-SQUIDs. The Si-Chip carrying the two SQUIDS is glued directly onto the noise source. Operating both SQUIDS in voltage biased mode in 2-stage SQUID configurations allows to reduce the power dissipation as well as the noise of the SQUIDS to a minimum. By computing the

cross-correlation of the two SQUID signals the noise contribution of the read-out is suppressed to a level which is marginal even at micro-Kelvin temperatures. To further increase the suppression we fabricated a new SQUID design with minimal mutual inductance of input and feedback coil. We compare the thermometer to a previously developed magnetic field fluctuation thermometer in the temperature range from 2.5 K down to 9 mK. Statistical uncertainties below 0.5 % are achieved within 10 s of measurement time. Within this uncertainty no self heating was observable at base temperature. This agrees with predictions from the thermal model of the thermometer, which suggests that self heating should be marginal even at temperatures well below 1 mK.

TT 71.3 Thu 15:30 HSZ 201

Development and Implementation of a New Compact Low-Noise Pulse Tube Cryocooler for Temperatures of 5 - 10 K — •Bernd Schmidt[1,2], Matthias Vorholzer[1,2], Marc Dietrich[1], 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, Justus-Liebig-University Giessen, Germany

Two-stage Pulse Tube Cryocoolers (PTC) are closed-cycle machines which provide cooling power near 4 K without the necessity of regularly buying and refilling Helium. In addition, PTC show lower intrinsic disturbances than other closed-cycle cryocoolers.

Since the invention of 4 K two-stage PTCs, further developments aimed at high cooling powers in order to compete with GM-cryocoolers. However, sensitive applications suffer from intrinsic disturbances of the cryocooler. To address this issue, the development of PTCs with small cooling powers is essential.

In this talk we present the development of a new two-stage GM-type PTC, designed to work with only 1 kW input power. After modeling the PTC, a first prototype was fabricated and then operated and optimized. Up to now, the PTC reaches a minimum temperature of about 4 K and provides a cooling power of 50 mW at 5 K, which is sufficient for cooling small cryoelectronic or optical devices. A comparison of the simulated and measured cooling performance will also be presented.

Funding via the BMBF joint project "SUSY" (grant No 13N13444) is gratefully acknowledged.

TT 71.4 Thu 15:45 HSZ 201

High efficiency thermoelectric devices based on superconductor-quantum dot hybrid — •Sun-Yong Hwang[1,2], Rosa Lopez[2], and David Sanchez[2] — [1]Theoretische Physik, Universitat Duisburg-Essen, D-47048 Duisburg, Germany — [2]Institut de Física Interdisciplinària i Sistemes Complexos IFISC (UIB-CSIC), E-07122 Palma de Mallorca, Spain

Superconductors are perfect electric conductors but poor thermal conductors which would be excellent for generating thermoelectric effects. However, the superconducting density of states exhibits particle-hole symmetry suppressing the thermovoltage creation. Therefore, one needs to devise a way to break this symmetry for thermoelectric applications. We propose that superconductor-quantum dot hybrid systems can pave the way for versatile thermoelectric devices with high efficiencies. By attaching a ferromagnetic lead to the quantum dot, this device can act as a thermoelectric engine with a large figure-of-merit ZT [1]. Moreover, nonlinear thermocurrents of this device show strong rectification and diode effects [2]. We also discuss interesting nonlinear cross coupling effects in the subgap regime [3]. Importantly, this device can be easily tunable by a gate potential and a magnetic field applied to the quantum dot.

[1] S.-Y. Hwang et al., Phys. Rev. B 94, 054506 (2016).
[2] S.-Y. Hwang et al., New J. Phys. 18, 093024 (2016).
[3] S.-Y. Hwang et al., Phys. Rev. B 91, 104518 (2015).

TT 71.5 Thu 16:00 HSZ 201

Silicon as an optical material for precision applications at cryogenic temperatures — •Rene Glaser[1], Stefanie Kroker[2], Johannes Dickmann[2], Carol B. Rojas-Hurtado[2], and Ronny Nawrodt[1] — [1]Friedrich-Schiller University Jena, Institute for Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]Physikalisch-Technische Bundesanstalt, Metrology for Functional Nanosystems, Bundesallee 100, 38116 Braunschweig, Germany

Silicon is a promising candidate material for precision instrumentation applications such as laser stabilization cavities or future interferometric gravitational wave detectors. Here, applications benefit from the low opto-mechanical noise and its excellent thermal properties.

We present a systematic study of optical properties of silicon-based optical components and show the influence of optical properties on the metrological applications. The focus of our studies lies on properties at 1550 nm in a wide temperature range from 4.2 K to 300 K.

TT 71.6 Thu 16:15 HSZ 201

Electric Field Dependence of Nuclear Quadrupole driven Relaxation in Glasses at Very Low Temperatures — •Annina Luck, Andreas Schaller, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, D-69120 Heidelberg

The universal behavior of amorphous solids at low temperatures, governed by two level tunneling systems and described by the standard tunneling model, has long been a generally accepted fact. Broadband dielectric measurements of glasses containing significant amounts of isotopes carrying very large nuclear electric quadrupole moments, have, however, revealed a relaxation mechanism involving nuclear spins, which is dominant at low frequencies and at temperatures below several hundred millikelvin. In particular, we have measured dielectric properties over eight orders of magnitude in frequency performed on the two multicomponent glasses N-KZFS11 and HY-1, containing significant amounts of tantalum and holmium respectively. As ^{181}Ta and ^{165}Ho both carry very large nuclear electric quadrupole moments, these glasses are ideal candidates to investigate the influence of these moments. In the regime where the nuclear spin enabled relaxation dominates, both glasses show a fundamentally different response to high electric fields, than observed in other glasses and predicted by theory. The observed saturation of the nuclear driven relaxation process at high fields allows a clear distinction between nuclear spin and phonon enabled effects and can help us gain a more detailed insight into the microscopic origin of the nuclear driven relaxation process.

15 min. break.

TT 71.7 Thu 16:45 HSZ 201

Development of a 64 pixel metallic magnetic calorimeter based detector array with integrated microwave SQUID multiplexer — •Mathias Wegner, Loredana Gastaldo, Andreas Fleischmann, Michael Keller, Daniel Richter, Sebastian Kempf, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, D-69120 Heidelberg

Microwave SQUID multiplexing (μMUXing) appears to be the most promising readout technique for arrays of low-temperature microcalorimeters requiring a large bandwidth per pixel. It is therefore highly suited for reading out metallic magnetic calorimeters (MMCs) that uniquely combine an intrinsically fast signal rise time, an excellent energy resolution and a highly linear detector response.

In this contribution we present the first demonstration of μMUXing of MMCs using a 64 pixel detector array that is read out by an integrated, on-chip multiplexer. Each detector features two 5 μm thick X-ray absorbers and is optimized for soft X-ray spectroscopy. The estimated energy resolution for all pixels within the array is below 10 eV. We will present our design and discuss a detailed characterization of the device. In particular, we will show that its performance is as expected when considering the geometry and the thermodynamical properties of the detectors as well as the multiplexer parameters. In addition, we will summarize the status of the development of a software defined radio based readout electronics as well as our advances concerning flux ramp modulation which we will use for linearizing the multiplexer output signal.

TT 71.8 Thu 17:00 HSZ 201

Development of a combined photon and phonon detector for rare-event experiments — •Clemens Hassel[1], Felix Ahrens[1], Christian Enss[1], Andreas Fleischmann[1], Loredana Gastaldo[1], Sebastian Kempf[1], Yong-Hamb Kim[2], Wonsik Yoon[2], Martin Loidl[3], Xavier-Francois Navick[3], and Matias Rodrigues[3] — [1]Kirchhoff-Institute for Physics, Heidelberg University, Germany. — [2]IBS Center for Underground Physics, Daejeon, Rep. of Korea — [3]CEA, Saclay, France.

Scintillating crystals in cryogenic experiments searching for a direct interaction of dark matter particles and for the neutrinoless double beta decay, as in AMoRE or LUMINEU, allow for an efficient active background reduction due to particle mass discrimination. This is achieved by the simultaneous measurements of heat and light generated by the interaction of a particle in the scintillating crystal. We are developing phonon and large area photon detectors based on metallic magnetic

calorimeters (MMCs) to readout both types of excitations. We will present the design for a photon detector P1 with an expected energy resolution of $\Delta E_{\mathrm{FWHM}} < 5$ eV and a signal rise time of $\tau < 50$ μs and discuss its fabrication and first experimental results. Furthermore we will present the design and the fabrication of the integrated photon and phonon detector P2, with a light detector inspired by P1 and three phonon sensors with $\Delta E_{\mathrm{FWHM}} < 100$ eV and $\tau < 200$ μs on the same chip. This allows for a very efficient readout, a minimum of material for support structures and further background reduction by position sensitive phonon signals.

TT 71.9 Thu 17:15 HSZ 201

Development of metallic magnetic micro-calorimeters for ECHo — •Dorothea Fonnesu for the ECHo-Collaboration — Kirchhoff-Institute for Physics, Heidelberg University, Germany.

The Electron Capture ^{163}Ho experiment ECHo aims to probe the electron neutrino mass on a sub-eV level via analysis of the calorimetrically measured electron capture spectrum of ^{163}Ho. For this metallic magnetic calorimeters (MMC) will be used, which are operated at millikelvin temperature. The performance achieved by first prototypes of MMC detector arrays with embedded ^{163}Ho already show that an energy resolution of $\Delta E_{\mathrm{FWHM}} < 3$eV and a signal rise time of $\tau < 1$ μs for ECHo can be reached. We present the current status of the detector developments for ECHo-1k, which is the first phase of the experiment with an activity of 1 kBq of the source and an expected sensitivity on the neutrino mass of below 10 eV. This includes the design and fabrication of the ECHo-1k detector and the necessary not standard fabrication processes to prepare the detector for the ion implantation of ^{163}Ho at RISIKO in Mainz. We also present simulations and experimental studies concerning the implantation process itself and measurements of the expected additional heat capacity of the detector due to the implantation of ^{163}Ho which is a crucial parameter for the detector performance.

TT 71.10 Thu 17:30 HSZ 201

SiM-X: The first step towards a large silicon microcalorimeter array — •Pascal Andree Scholz[1], Victor Andrianov[2], Artur Echler[3,4], Peter Egelhof[3,4], Oleg Kiselev[3], Saskia Kraft-Bermuth[1], and Damian Muell[1] — [1]Justus-Liebig-Universität, Giessen, Germany — [2]Lomonosov Moscow State University, Moscow, Russia — [3]GSI Helmholtz Center, Darmstadt, Germany — [4]Johannes-Gutenberg Universität, Mainz, Germany

High-precision X-ray spectroscopy of highly-charged heavy ions provides a sensitive test of quantum electrodynamics in very strong Coulomb fields. Due to their excellent energy resolution for X-ray energies around 100 keV, silicon microcalorimeters, based on silicon thermistors and tin absorbers, have already demonstrated their potential to improve the precision in previous experiments at the Experimental Storage Ring (ESR) of the GSI Helmholtz Center for Heavy Ion Research. In june 2016 a new compact detector design along with a new cryogen-free cryostat equipped with a pulse tube cooler was applied in a test experiment at the ESR. This test was an important benchmark for designing a larger detector array with three times the active detector area, which is currently in preparation, and, thus, with an improved lateral sensitivity and statistical accuracy. In this presentation, we will introduce the ESR test experiment following results and discuss current developments and potential future applications.

TT 71.11 Thu 17:45 HSZ 201

Application of Calorimetric Low Temperature Detectors for the Investigation of Z-Yield Distributions of Fission Fragments — •Santwana Dubey[1,2], Shawn Bishop[4], Aurelien Blanc[5], Johannes O. Denschlag[2], Artur Echler[1,2], Peter Egelhof[1,2], Friedrich Goennenwein[6], Jose Gomez[4], Patrick Grabitz[1,2], Ulli Koester[5], Saskia Kraft-Bermuth[3], Werner Lauterfeld[2], Manfred Mutterer[1], Pascal Scholz[3], and Stefan Stolte[2] — [1]GSI, Germany — [2]Univ. Mainz, Germany — [3]Univ. Giessen, Germany — [4]Technical Univ. Munich, Germany — [5]ILL Grenoble, France — [6]Univ. Tübingen, Germany

Precise fission fragment yield data are of great interest for a better understanding of the fission process. In a recent experiment, performed at the research reactor ILL Grenoble, Calorimetric Low Temperature Detectors (CLTDs) were applied for the first time for the investigation of Z-yield distributions of fission fragments. Fission fragments, produced by thermal neutron induced fission of 235U, were passed through the LOHENGRIN separator to filter required mass and energy, followed by SiN degrader foils to separate elements with different Z within a mass, and were detected on an array of CLTDs. Preliminary data for the mass region 82<A<132 will be presented, which would lead to a better understanding of the fission process, as well as of reactor neutrino oscillations and the reactor neutrino anomaly.

TT 72: Correlated Electrons: Frustrated Magnets - General 2

Time: Thursday 15:00–18:30 Location: HSZ 204

TT 72.1 Thu 15:00 HSZ 204

The role of nonmagnetic d0 vs d10 B-type cations on the magnetic exchange interactions in osmium double perovskites — •Hai Feng[1], Kazunari Yamaura[2], Martin Jansen[3], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids — [2]National Institute for Materials Science — [3]Max Planck Institute for Solid State Research

Double perovskite oxides, A2BB'O6, containing 4d/5d elements have attracted considerable attention due to their remarkable electronic and magnetic properties, such as room-temperature magnetoresistance and high-temperature ferrimagnetism. In this talk, we will present our studies on the magnetic properties of osmium double perovskite oxides Ba2BOsO6 (B = Sc, Y, In). Ba2BOsO6 (B = Sc, Y, In) adopt the cubic double perovskite structures (space group, Fm-3m) with ordered B and Os arrangements and show antiferromagnetic transitions at 93 K, 69 K, and 28 K, respectively. The Weiss-temperatures are -590 K for Ba2ScOsO6, -571 K for Ba2YOsO6, and -155 K for Ba2InOsO6. Sc3+ and Y3+ have the open-shell d0 electronic configuration, while In3+ has the closed-shell d10. This indicates that a d0 B-type cation induces stronger overall magnetic exchange interactions in comparison to a d10. Comparison of Ba2BOsO6 (B = Sc, Y, In) to their Sr and Ca analogues shows that the structural distortions weaken the overall magnetic exchange interactions.

TT 72.2 Thu 15:15 HSZ 204

Magnetic properties of A_2TaCl$_6$ with $5d^1$ electons on FCC lattice — •Hajime Ishikawa[1], Tomohiro Takayama[2], Robert Dinnebier[2], and Hidenori Takagi[2] — [1]University of Stuttgart, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

$5d$ transition metal compounds are expected to show exotic magnetism as a result of the interplay between electronic correlation and strong spin-orbit coupling. In the case of $5d^1$ electronic configuration, the electron is considered to occupy the $J_{eff} = 3/2$ states, where effective orbital angular momentum $L_{eff} = 1$ and spin angular momentum $S = 1/2$ cancel with each other. In recent theoretical studies, rich ground states are predicted in the system where localized electrons in $J_{eff} = 3/2$ states are arranged on the face centered cubic (FCC) lattice. Experimentally, several double perovskite oxides with FCC lattice have been studied as a model compound, however, their spin and orbital states are still unclear and under debate. The FCC lattice made of transition metal ions are also found in a series of halides with the chemical formula A_2MX_6. In this study, we studied physical properties of A_2TaCl$_6$ with $5d^1$ electronic configuration and their related materials by means of magnetization and heat capacity measurements and low-temperature X-ray diffraction experiments. Based on the results, we discuss the spin-orbital state of Ta^{4+} ion and difference between oxides and halides.

TT 72.3 Thu 15:30 HSZ 204

ESR Spectroscopy on the Coupled Spin Tetrahedral System $Cu_2Te_2O_5Cl_2$ — •Julian Zeisner[1,2], Vladislav Kataev[1], Mirta Herak[3], Dijana Zilic[4], Helmuth Berger[5], and Bernd Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, Germany — [3]Institute of Physics, Zagreb, Croatia — [4]Rudjer Boskovic Institute, Zagreb, Croatia — [5]Institut de Physique de la Matière Complexe, EPFL, Lausanne, Switzerland

Systems with reduced dimensionality and magnetic frustration gained considerable attention in modern solid state research as both phenomena individually lead to an enhancement of the impact of fluctuations on magnetic properties and low-energy excitations. The coupled spin tetrahedral compound $Cu_2Te_2O_5Cl_2$ belongs to a class of materials which allow to study the interplay of both effects. In our work we performed a high-field high-frequency ESR study in order to investigate the magnetic anisotropies present in this system as well as the spin dynamics of the compound. Measurements were conducted over a wide frequency and temperature range revealing a small g-factor anisotropy at room temperature which is consistent with torque magnetometry results. Furthermore, the temperature dependence of the linewidth indicates the onset of slowing down of spin fluctuations far above the ordering temperature.

TT 72.4 Thu 15:45 HSZ 204

J_1-J_2 Heisenberg model on a triangular-lattice bilayer — •Darshan G. Joshi[1] and Matthias Vojta[2] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

We consider a triangular-lattice bilayer Heisenberg model for spins 1/2 with antiferromagnetic nearest-neighbor and next-nearest-neighbor interactions. We determine the phase diagram and the dispersion of elementary excitations using variants of bond-operator theory. Large inter-layer coupling yields a dimer quantum paramagnet, while magnetic order is possible for weak inter-layer coupling. Frustration can induce flat portions of triplon bands in the dimer phase, opening the window to find exotic states in the vicinity to the transition point to ordered phases. For weak inter-layer coupling we reproduce the possible spin-liquid state known from the single-layer J_1-J_2 model which occurs when 120° order is destroyed by increasing J_2. Remarkably, this state is destabilized in favor of magnetic order with increasing inter-layer coupling before amplitude fluctuations destroy magnetic order at large inter-layer coupling.

TT 72.5 Thu 16:00 HSZ 204

Quantum domain walls induce incommensurate supersolid phase on the anisotropic triangular lattice — •Xue-Feng Zhang[1,2], Shijie Hu[2], Axel Pelster[2], and Sebastian Eggert[2] — [1]Max-Planck- Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Physics Department and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

We investigate the extended hard-core Bose-Hubbard model on the triangular lattice as a function of spatial anisotropy with respect to both hopping and nearest-neighbor interaction strength [1]. At half filling the system can be tuned from decoupled one-dimensional chains to a two-dimensional solid phase with alternating density order by adjusting the anisotropic coupling. At intermediate anisotropy, however, frustration effects dominate and an incommensurate supersolid phase emerges, which is characterized by incommensurate density order as well as an anisotropic superfluid density. We demonstrate that this intermediate phase results from the proliferation of topological defects in the form of quantum bosonic domain walls. Accordingly, the structure factor has peaks at wave vectors, which are linearly related to the number of domain walls in a finite system in agreement with extensive quantum Monte Carlo simulations. We discuss possible connections with the supersolid behavior in the high-temperature superconducting striped phase.

[1] Phys. Rev. Lett. 117, 193201 (2016)

TT 72.6 Thu 16:15 HSZ 204

Character of the Néel Transition of Triangular Antiferromagnet $PdCrO_2$ — •Jack Bartlett[1,2], Dan Sun[1], Jhuma Sannigrahi[1], Pallavi Kushwaha[1], Andrew Mackenzie[1,2], and Clifford Hicks[1] — [1]Max-Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, Dresden, 01187, Germany — [2]Scottish Universities Physics Alliance (SUPA), School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS, United Kingdom

The transition from paramagnetism to antiferromagnetism is usually second-order, but can be driven first-order through magnetoelastic coupling or fluctuation effects. In this talk, we present data on the antiferromagnetic transition of $PdCrO_2$. This is a layered, triangular compound consisting of alternating sheets of highly conductive Pd and insulating, magnetic CrO_2. The Cr spins are Heisenberg-like, and below T_N ∼38 K order into the the 120° Néel phase. Resistivity data on uniaxially-stressed $PdCrO_2$ suggest that at zero stress the transition is weakly first-order, however on close inspection the transition appears to be a crossover. We discuss further using resistivity, thermal expansion, and susceptibility data.

TT 72.7 Thu 16:30 HSZ 204

The response of a triangular antiferromagnet to anisotropic lattice distortion — •Dan Sun[1], Jack Bartlett[1,2], Jhuma Sannigrahi[1], Pallavi Kushwaha[1], Andrew Mackenzie[1,2], and Clifford Hicks[1,2] — [1]Max-Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, Dresden, 01187, Germany — [2]Scottish Universities Physics Alliance (SUPA), School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS, United Kingdom

The ground state of Heisenberg spins interacting antiferromagnetically on a triangular lattice is 120° antiferromagnetic order. We probe the effects of anisotropic lattice distortion on this phase using the material $PdCrO_2$, which has highly-conducting Pd sheets that alternate with Mott-insulating CrO_2 layers. The Cr spins order into a 120° phase at T_N = 39 K. The conductivity of the Pd sheets can be measured to probe magnetic scattering across the transition. In the unstrained lattice, the resistivity has a sharp first-order-like step at T_N. It persists with almost no change up to a compression of ∼ 0.2%, then broadens dramatically. This feature suggests a rigidity of the 120° phase at T ∼ T_N against small perturbations, which we discuss in terms of magnetoelastic coupling and fluctuation effects.

15 min. break.

TT 72.8 Thu 17:00 HSZ 204

Non-Abelian Symmetries in Tensor Network Algorithms — •Philipp Schmoll[1,2] and Román Orús[1] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany

In recent years Tensor Networks (TNs) have emerged as a natural language to describe quantum states of matter by capturing the amount and local structure of entanglement in the system. They provide an efficient framework to study quantum many-body properties with many remarkable applications such as the Density Matrix Renormalization Group (DMRG) for 1d systems proposed by S. White. The Projected Entangled Pair State (PEPS) ansatz has proven to be a versatile tool for 2d systems with topological order, both chiral and non-chiral. However, at the current stage simulations in 2d are strongly limited due to the complexity of the systems. In this respect, a big step needs to be taken to have a versatile implementation of non-abelian symmetries (such as SU(2) or SU(3)) in 2d PEPS algorithms, which will allow to advance significantly in the study of many relevant systems (e.g., frustrated antiferromagnets, chiral topological spin liquids, ...). In this talk I will report on recent advances in this direction at our group in Mainz.

TT 72.9 Thu 17:15 HSZ 204

The spin-1/2 Kagome XXZ model in a field: competition between lattice nematic and solid orders — •Augustine Kshetrimayum[1], Thibaut Picot[2], Román Orús[1], and Didier Poilblanc[2] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Laboratoire de Physique Théorique, IRSAMC, CNRS and Université de Toulouse, UPS, F-31062 Toulouse, France

We study numerically the spin-1/2 XXZ model in a field on an infinite Kagome lattice. We use different algorithms based on infinite Projected Entangled Pair States (iPEPS) for this, namely: (i)an approach with simplex tensors and 9-site unit cell, and (ii) an approach based on coarse-graining three spins in the Kagome lattice and mapping it to a square-lattice model with local and nearest-neighbor interactions, with usual PEPS tensors, 6- and 12-site unit cells. We observe the emergence of several magnetization plateaus as a function of the field for different values of the anisotropy. We focus on the 1/3 plateaus using both the techniques and study the nature of its ground state as we tune the anisotropy from the Ising regime to the XY regime through the Heisenberg point and find a strong competition between lattice nematic and solid orders.

TT 72.10 Thu 17:30 HSZ 204

Magnetic properties of Li_2FeSiO_4 single crystals — •Fabian Billert, Johannes Werner, Christoph Neef, Changhyun Koo, and Rüdiger Klingeler — Kirchhoff Institute of Physics, Heidelberg

University, Heidelberg

Li_2FeSiO_4 single crystals of the high-temperature *Pmnb*-phase were grown by means of the travelling-solvent floating-zone technique. The single-crystal structure refinement reveals corner-sharing FeO_4 and SiO_4 tetrahedra in the *ac*-layers. Static magnetisation studies reveal long-range antiferromagnetic order below $T_N = 17$ K. The maximum of the magnetic suceptibility appears at around 25 K indicating significant antiferromagnetic correlations well above T_N. This is corroborated by means of high-frequency electron spin resonance (HF-ESR) measurements which show temperature dependent resonances, i.e. the evolution of local magnetic fields, up to 100 K. Below T_N, antiferromagnetic resonance modes are detected and significant zero-field splitting is observed.

TT 72.11 Thu 17:45 HSZ 204

Strong coupling on structure and magnetism in $SrCo_2P_2$ — •Inga Kraft[1,2], Kathrin Götze[3,2], Johannes Klotz[3], Vivien Lorenz[4], Christoph Bergmann[1], Yurii Prots[1], Jan Bruin[5], Alix McCollam[5], Ilya Sheikin[6], Jochen Wosnitza[2], Christoph Geibel[1], and Helge Rosner[1] — [1]MPI CPfS, Dresden — [2]Technical University of Dresden — [3]HLD-EMFL, Dresden — [4]Institut für Festkörper- und Werkstoffforschung (IFW), Dresden — [5]HFML-EMFL, Nijmegen, The Netherlands — [6]CNRS Grenoble, France

Though the iron pnictide 122 systems show a comparatively simple structure, they attracted large interest owing to their rich physics. $SrCo_2P_2$ is closely related to the iron-pnictide superconductors, but does not show superconductivity or magnetic order down to 300 mK. In contrast, previous DFT band structure calculations found a large DOS at E_F and predicted a magnetic (or other) instability. Based on new low temperature XRD structural data, we calculate the respective electronic structure and compare it to the angle-dependent dHvA measurements. Our results yield a strongly reduced DOS(E_F) and explain the observed strong magnetic fluctuations and absence of magnetic order.

TT 72.12 Thu 18:00 HSZ 204

Spin liquid and quantum phase transition without symmetry breaking in a frustrated three-dimensional Ising model — •Kai Phillip Schmidt[1], Julia Roechner[2], and Leon Balents[3] — [1]FAU Erlangen-Nürnberg, Erlangen, Germany — [2]TU Dortmund, Dortmund, Germany — [3]Kavli Institute for Theoretical Physics, University of California, Santa Barbara, USA

We show that the highly frustrated transverse-field Ising model on the three-dimensional pyrochlore lattice realizes a first-order phase transition without symmetry breaking between the low-field Coulomb quantum spin liquid and the high-field polarized phase. The quantum phase transition is located quantitively by comparing low- and high-field series expansions. Furthermore, the intriguing properties of the elementary excitations in the polarized phase are investigated. We argue that this model can be achieved experimentally by applying mechanical strain to a classical spin ice material comprised of non-Kramers spins such as $Ho_2Ti_2O_7$. Taken together with our results, this provides a new experimental platform to study quantum spin liquid physics.

TT 72.13 Thu 18:15 HSZ 204

Magnetism of correlated covalent insulator $SrRu_2O_6$ — Atsushi Hariki and •Jan Kuneš — TU Wien, Austria

We present a density functional + dynamical mean-field theory (LDA+DMFT) study of $SrRu_2O_6$. Considering the interaction strength this d^3 material is on the correlated-metal side of the Mott transition. Special hopping pattern, however, gives rise to pronounced molecular orbital features and results in opening of a hybridization gap. The physics is governed by a competition between localization and covalency in a half-filled Hund's material.

TT 73: Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 2

Time: Thursday 15:00–18:00 Location: HSZ 304

TT 73.1 Thu 15:00 HSZ 304

Study of dynamical localization in interacting Floquet systems — •Tibor Rakovszky[1], Frank Pollmann[1], Curt von Keyserlingk[2], and Shivaji Sondhi[3] — [1]Physik-Department, Technische Universität München, D-85748 Garching, Germany — [2]Princeton Center for Theoretical Science, Princeton University, Princeton, New Jersey 08544, USA — [3]Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

Since the seminal work of Fishman, Grempel and Prange on the kicked rotator[1], it is known that periodically driven - otherwise known as Floquet - systems can exhibit 'dynamical localization': a variant of Anderson localization in which the particle is localized not in real, but in momentum space. In the past decade it became clear that Anderson localization in real space is robust against sufficiently weak interactions, leading to a phenomenon called many-body localization. It is therefore a natural question to ask whether the dynamical localization, exhibited by periodically driven free particles, also has an interacting analogue. In this talk we review recent results regarding this question and compare them to our own results acquired through large-scale numerical simulations.
[1] S. Fishman, D.R. Grempel and R.E. Prange, Phys. Rev. Lett. 49, 509 (1982)

TT 73.2 Thu 15:15 HSZ 304

Spatiotemporal buildup of density-density correlations in the 2d Hubbard model — •Manuel Kreye and Stefan Kehrein — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

Driven by recent experimental advances in ultracold atomic gases, the dynamical behavior of quantum many-body systems far from equilibrium has gained a lot of interest. The theoretical comprehension of the observations and the prediction of new phenomena require powerful and reliable methods for studying the real-time dynamics of these many-body systems.

In this work, we apply the method of unitary perturbation theory to study the spatiotemporal buildup of density-density correlations in the two-dimensional Hubbard model after a weak interaction quench. We present analytical results for both susceptibilities and correlation functions on all time scales.

TT 73.3 Thu 15:30 HSZ 304

Spatiotemporal correlation build-up after an interaction quench in the Luttinger model — •Nils O. Abeling, Markus Schmitt, Manuel Kreye, and Stefan Kehrein — Institut für Theoretische Physik, Georg-August-Universität, Göttingen

We study the evolution of density-density correlations at different times and distances in the exactly solvable Luttinger model after a sudden quench from the ground state. We discuss the difference between correlations and susceptibilities, and how these results can be interpreted from the point of view of Lieb-Robinson bounds. For the correlation functions we specifically show that pre-quench entanglement in the ground state leads to algebraically decaying long distance tails outside the light cone.

TT 73.4 Thu 15:45 HSZ 304

Transport dynamics in a quenched tunnel-coupled Luttinger liquid — •Filippo M. Gambetta[1], Fabio Cavaliere[1], Maura Sassetti[1], Alessio Calzona[1,2], Roberta Citro[3], and Matteo Carrega[4] — [1]Università di Genova and SPIN-CNR, Genova, Italy — [2]University of Luxembourg, Luxembourg — [3]Università di Salerno and SPIN-CNR, Fisciano (SA), Italy — [4]NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Pisa, Italy

The transport dynamics of a quenched Luttinger liquid tunnel-coupled to a fermionic non-interacting probe is investigated. In the transient dynamics, we show that for a sudden quench of the electron interaction universal power-law decay in time of the tunneling current occurs, ascribed to the presence of entangled compound excitations created by the quench. In sharp contrast to the usual nonuniversal power-law behavior of a zero-temperature nonquenched Luttinger liquid, the steady-state tunneling current is Ohmic and can be explained in terms of an effective quench-activated heating of the system. Furthermore, by studying the fractionalization of charge and energy injected through the tunneling junction, we demonstrate that in the steady state the charge fractionalization ratio is unaffected by the pre-quenched pa-

rameters. On the contrary, due to the post-quench non-equilibrium spectral function, the energy partitioning ratio is strongly modified, reaching values even larger than one. This is a peculiar feature of the non-equilibrium dynamics of the quench process and it is in sharp contrast with the non-quenched case, where the ratio is bounded by one.

TT 73.5 Thu 16:00 HSZ 304

Out-of-equilibrium density dynamics of a quenched fermionic system — •Sergio Porta[1], Filippo M. Gambetta[1,2], Fabio Cavaliere[1,2], Niccolò Traverso Ziani[3], and Maura Sassetti[1,2] — [1]Università di Genova, Genova, Italy — [2]SPIN-CNR, Genova, Italy — [3]University of Würzburg, Würzburg, Germany

Using a Luttinger liquid theory we investigate the time evolution of the particle density of a one-dimensional fermionic system with open boundaries and subject to a finite duration quench of the inter-particle interaction. We provide analytical and asymptotic solutions to the unitary time evolution of the system, showing that both switching on and switching off the quench ramp create light-cone perturbations in the density. The post-quench dynamics is strongly affected by the interference between these two perturbations. In particular, we find that the discrepancy between the time-dependent density and the one obtained by a generalized Gibbs ensemble picture vanishes with an oscillatory behavior as a function of the quench duration, with local minima corresponding to a perfect overlap of the two light-cone perturbations. For adiabatic quenches, we also obtain a similar behavior in the approach of the generalized Gibbs ensemble density towards the one associated with the ground state of the final Hamiltonian.

TT 73.6 Thu 16:15 HSZ 304

Multiple particle-hole pair creation in the Fermi-Hubbard model — Nicolai ten Brinke, Manuel Ligges, Uwe Bovensiepen, Ralf Schützhold, and •Friedemann Queisser — Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße, Duisburg 47048, Germany

We study the Fermi-Hubbard model in the strongly correlated Mott phase under the influence of a harmonically oscillating hopping rate $J(t) = J_0 + \triangle J \cos(\omega t)$ [1]. Apart from the well-known fundamental resonance where the frequency ω of this oscillation equals (or a little exceeds) the Mott gap, we also find higher-order resonances where multiple particle-hole pairs are created when ω is near an integer multiple of the gap. These findings should be relevant for experimental realizations such as ultra-cold fermionic atoms in optical lattices or pump-probe experiments using laser pulses incident on correlated electrons in solid state materials.

[1] N. ten Brinke, M. Ligges, U. Bovensiepen and R. Schützhold, arXiv:1602.00871

15 min. break.

TT 73.7 Thu 16:45 HSZ 304

The nature of the pressure-induced metallization in VO_2 — •Johannes M. Braun[1,2], Harald Schneider[1], Manfred Helm[1,2], Rafał Mirek[3], Lynn A. Boatner[4], Robert E. Marvel[5], Richard F. Haglund[5], and Alexej Pashkin[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]TU Dresden, Germany — [3]University of Warsaw, Poland — [4]Oak Ridge National Laboratory, USA — [5]Vanderbilt University, Nashville, USA

We utilize ultrafast optical pump – THz probe spectroscopy in order to investigate the pressure-driven insulator-to-metal transition (IMT) in vanadium dioxide (VO_2). The probe pulses with central frequency of 30 THz enable a sensitive detection of the photoinduced metallization.

The threshold pump fluence necessary for generation of a metastable metallic phase has been systematically measured for pressures up to 19 GPa. Initial pressure application leads to a notable increase of the threshold fluence. This contrasts the thermally-driven IMT in VO_2 where it decreases on approaching the transition temperature. Above the IMT, that occurs at approximately 6–8 GPa, we observe a sharp drop of the threshold fluence. However, the clear threshold behavior characteristic for systems with cooperative electronic localization still could be observed also in the metallic state up to the highest applied pressure.

Our results support a view of the pressure-induced IMT in VO_2 as a purely electronic bandwidth-driven Mott-Hubbard transition, that does not involve any change in the crystal structure.

TT 73.8 Thu 17:00 HSZ 304

Coherent Order Parameter Oscillations in the Ground State of the Excitonic Insulator Ta_2NiSe_5 — •Daniel Werdehausen[1,2], Tomohiro Takayama[1,2], Marc Höppner[1], Gelon Albrecht[1,2], Andreas W. Rost[1,2], Yangfan Lu[3], Dirk Manske[1], Hidenori Takagi[1,2], and Stefan Kaiser[1,2] — [1]Max Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]Universität Stuttgart, Germany — [3]University of Tokyo, Japan

The excitonic insulator state is an intriguing correlated electron phase that consists of condensed excitons. However, its experimental identification has proven to be challenging, mainly because it is difficult to probe the coherence of a condensate directly. One possibility is the observation of a condensate's intrinsic collective modes, which are equivalent to the Higgs- and Goldstone modes in superconductors. Here we report strong evidence for the existence of an excitonic insulator state in Ta_2NiSe_5: Using non-linear excitations with short laser pulses we identify a phonon-coupled state of the exciton condensate, in which its electronic Higgs-mode couples to a low frequency phonon [1]. The Higgs-mode contribution substantiates the picture of an electronically driven phase transition and can be used to characterize the transient order parameter of the excitonic insulator as a function of temperature and excitation density.

[1] D. Werdehausen et al. arxiv:1611.01053 (2016).

TT 73.9 Thu 17:15 HSZ 304

Real-time broadening of non-equilibrium density profiles and the role of the specific initial-state realization — •Robin Steinigeweg[1], Fengping Jin[2], Daniel Schmidtke[1], Hans De Raedt[3], Kristel Michielsen[2,4], and Jochen Gemmer[1] — [1]University Osnabrück — [2]Forschungszentrum Jülich — [3]University Groningen — [4]RWTH Aachen University

The real-time broadening of density profiles starting from non-equilibrium states is at the center of transport in condensed-matter systems and dynamics in ultracold atomic gases. Initial profiles close to equilibrium are expected to evolve according to linear response, e.g., as given by the current correlator evaluated exactly at equilibrium. Significantly off equilibrium, linear response is expected to break down and even a description in terms of canonical ensembles is questionable. We unveil [1] that single pure states with density profiles of maximum amplitude yield a broadening in perfect agreement with linear response, if the structure of these states involves randomness in terms of decoherent off-diagonal density-matrix elements. While these states allow for spin diffusion in the XXZ spin-1/2 chain at large exchange anisotropies, coherences yield entirely different behavior.

[1] R. Steinigeweg et al., arXiv:1610.05778 (2016).

TT 73.10 Thu 17:30 HSZ 304

Time evolution of two holes in $t-J$ chains with anisotropic couplings — •Salvatore R. Manmana[1], Holger Thyen[1], Thomas Köhler[1], and Stephan C. Kramer[1,2] — [1]Institut f. Theoretische Physik, U. Göttingen — [2]Fraunhofer ITWM Kaiserslautern

Using time-dependent Matrix Product State (MPS) methods we study the real-time evolution of hole-excitations in $t-J$ chains close to filling $n = 1$. The dynamics in 'standard' $t-J$ chains with SU(2) invariant spin couplings is compared to the one when introducing anisotropic, XXZ-type spin interactions as realizable, e.g., by ultracold polar molecules on optical lattices. The simulations are performed with MPS implementations based on the usual singular value decompositions (SVD) as well as ones using the adaptive cross approximation (ACA) instead. The ACA can be seen as an iterative approach to SVD which is often used, e.g., in the context of finite-element-methods, leading to a substantial speedup. A comparison of the performance of both algorithms in the MPS context is discussed.

Financial support via DFG CRC 1073 "Atomic scale control of energy conversion", project B03, is gratefully acknowledged.

TT 73.11 Thu 17:45 HSZ 304

Time-resolved correlation functions of the BEC/BCS crossover from many-body Ramsey interferometry — •Johannes Oberreuter[1], Henning Moritz[2], and Michael Knap[1] — [1]Department of Physics, Walter Schottky Institute and Institute for Advanced Study, Technical University of Munich, 85748 Garching, Germany — [2]Institut für Laserphysik, University of Hamburg, 22761 Hamburg, Germany

We propose a local and time-resolved probe to study the BEC/BCS crossover. The protocol is based on Ramsey interferometry between

the two participating hyperfine states. We study rotations within the spin components as the third level typically suffers from increased loss. While on the BEC side the local spatial resolution cannot resolve the tightly bound molecules, on the BCS side as well as near unitarity we obtain dynamical information about the relevant scales.

TT 74: Graphene: Electronic Properties, Structure and Substrate Interaction II (joint session DY, DS, HL, MA, O, TT, organized by O)

Time: Thursday 15:00–18:15 Location: TRE Ma

TT 74.1 Thu 15:00 TRE Ma

Microscopic investigations of graphene grown on copper foil — •Philip Schädlich[1], Florian Speck[1], Julia Krone[1], Patrick Herlinger[2], Pranoti Kshirsagar[2], Martina Wanke[1], Jurgen Smet[2], and Thomas Seyller[1] — [1]Professur für Technische Physik, TU Chemnitz, Reichenhainer Straße 70, D-09126 Chemnitz, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

Graphene grown by CVD on polycrystalline copper foil is investigated by PEEM, LEEM, LEED and STM. LEED indicates that the flakes consist of rotated domains as well as twisted bilayer areas. The twist between two graphene layers grown on top of each other leads to the formation of periodic Moiré superstructures, which were observed by STM. In addition, the formation of surface facets on the copper foil gives rise to a stripe pattern in PEEM and LEEM, and a displaced LEED pattern, which can be attributed to the inclined terraces of the faceted surface by dark field LEEM. Inclination angles between facets have been determined by energy dependent LEED and are comparable with literature reports [1, 2]. AFM and STM confirm the results of the faceted surface obtained by LEEM.

[1] S. Nie, et al., New J. Phys. **14**, 093028 (2012).
[2] J. Kraus, et al., Carbon **64**, 377 (2013).

TT 74.2 Thu 15:15 TRE Ma

Local electronic properties of the graphene-protected giant Rashba-split $BiAg_2$ surface — •Julia Tesch[1], Milan Jubitz[1], Elena Voloshina[2], Yuriy Dedkov[1], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Institut für Chemie, Humboldt-Universität zu Berlin, 10099 Berlin, Germany

In search of future spintronic devices, combined systems of graphene and strongly Rashba-split surfaces, such as the heavy post-transition and noble metal surface alloy $BiAg_2$, have become of particular interest.

Following a detailed discussion of the challenging yet well reproducible sample fabrication technique that allows us to fine tune the properties of the resulting system, we present a comprehensive study of the gr/$BiAg_2$ structure by means of scanning tunnelling microscopy as well as spectroscopy supported by density functional theory calculations. Besides the persistent relativistic nature of graphene charge carriers upon adsorption, we report on a downward shift of the preserved $BiAg_2$ surface state. This peculiar phenomenon can be explained by an inward relaxation of Bi atoms into the underlying thick Ag layer and thus a subsequent delocalisation of the surface state wavefunction. Despite the close proximity of the giant Rashba-split surface to graphene, no spin splitting has been observed in graphene in both experiment and theory, while the spin-texture of $BiAg_2$ remains intact protected by graphene adsorption making this system a promising candidate for spintronic applications.

TT 74.3 Thu 15:30 TRE Ma

Controlling intramolecular hydrogen-transfer by electrostatic doping using gate-tunable STM — •Shai Mangel[1], Christian Dette[1], Katharina Polyudov[1], Paul Punke[1], Roberto Urcuyo[1], Marko Burghard[1], Soon Jung Jung[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, D-70569 Stuttgart — [2]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Electron transport properties can be controlled by intramolecular reactions that reshape the electronic configuration without changing the conformation. A prominent example is tautomerization, i.e. the interconversion between two isomers due to migration of hydrogen, which can be induced by STM. Several methods to control the tautomerization reaction were developed, such as depositing adatoms or using thermal and photoinduced excitation. However, those methods are usually limited in their spatial range and not always reversible. In this work, we demonstrate a global control of the electron density surrounding H_2-phthalocyanine on graphene/SiO_2/Si. By using a gate-tunable STM, we electrostatically doped the graphene substrate altering the chemical potential in the molecules surrounding, which results in up to 60% decrease of the tautomeric switching rate. This reduction is assigned to an increase in the energetic barrier of the tautomerization reaction. Understanding and controlling the electric field-effect on molecules via modification of the chemical potential of graphene is critical for designing future molecular electronic devices.

TT 74.4 Thu 15:45 TRE Ma

Structure of pristine and hBN-embedded graphene quantum dots on Ir(111) — •Jiaqi Cai[1], Caio Silva[1,2], Wouter Jolie[2], Ferdinand Farwick zum Hagen[2], Christoph Schlueter[3], Tien-Lin Lee[3], and Carsten Busse[1,2] — [1]Institut für Materialphysik, Münster, Germany — [2]II. Physikalisches Institut, Köln, Germany — [3]Diamond Light Source Ltd, Didcot, United Kingdom

Nanometer-sized graphene flakes (graphene quantum dots, GQDs) provide a playground for the confinement of Dirac electrons [1]. On Ir(111), these GQDs are dome-shaped, with their edges bend towards and strongly bond to Ir surface atoms [2]. We prepare GQDs with an average size of 2 nm, and explore the details of the varying graphene-substrate interaction with the x-ray standing wave technique. We precisely measure the bond distances of the C atoms at the edges as well as in the interior of the GQDs.

In order to stabilize these graphene nanostructures and to reach a well-defined edge termination, we embedded the GQDs in hexagonal boron nitride (hBN). We investigate the structural changes caused by the embedding, especially at the graphene-hBN interface, where peculiar electronic effects, such as half-metallicity are predicted [3]. The GQDs edges remain strongly bonded to the substrate, and the interface is comprised of both N-C and B-C bonds.

[1] W. Jolie et al., Phys. Rev. B 89, 155435 (2014).
[2] P. Lacovig et al., Phys. Rev. Lett. 103, 166101 (2009).
[3] S. Dutta et al., Phys. Rev. Lett. 102, 096601 (2009).

TT 74.5 Thu 16:00 TRE Ma

Investigation of Graphene using Simultaneous Scanning Tunneling/Atomic Force Microscopy — •Majid Fazeli Jadidi and Hakan Özgür Özer — Istanbul Technical University, Istanbul, Turkey

We investigated graphene layers grown on Cu foils using simultaneous Scanning Tunneling Microscopy/Atomic Force Microscopy (STM/AFM). Atomic resolution images of the surface were obtained in many channels such as STM topography, oscillation amplitude, force, tunnel barrier height and phase shift. The simultaneous acquisition of multiple channels allows us to compare images at every pixel, which in turn sheds light on the contrast mechanisms in probe microscopy. In HOPG or multilayer graphene, due to the shift between two successive layers, 3 atoms of the hexagon have an atom underneath (alpha (A) site) whereas the other 3 don't have (beta (B) site). Hence, three main atomic structures at the surface are A and B atoms and hollow sites. In STM images B atoms appear higher due to the dominance of their electronic structure over A site atoms. In the oscillation amplitude images which is a measure of the interaction stiffness[1], the brighter spots match with the A sites. The oscillation amplitude throughout the entire image is well below the free amplitude which suggests a very high positive interaction stiffness. This observation is supported also by the Force-distance spectroscopy which is simultaneously acquired with all such acquisition channels.

[1] A. Oral, R. A. Grimble, H. Ö. Özer, P. M. Hoffmann, and J. B. Pethica, Appl. Phys. Lett. 79, 1915 (2001).

TT 74.6 Thu 16:15 TRE Ma

Strong electron-phonon coupling in the σ band of graphene — Federico Mazzola[1], Thomas Frederiksen[2], Thiagarajan Balasubramanian[3], Philip Hofmann[4], •Bo Hellsing[5], and Justin W. Wells[1] — [1]Department of Physics, Norwegian University of Science and Technology (NTNU), Trondheim, Norway — [2]Donostia International Physics Center (DIPC) – UPV/EHU, San Sebastián, Spain — [3]MAX IV Laboratory, Lund, Sweden — [4]Department of Physics, Aarhus University, Denmark — [5]Department of Physics, University of Gothenburg, Sweden

First-principles studies of the electron-phonon coupling in graphene predict a high coupling strength for the σ band with values of the dimensionless mass-enhancement parameter λ up to 0.9. Near the top of the σ band λ is found to be ≈ 0.7. This value is consistent with the observed kink in the σ band dispersion near the $\bar{\Gamma}$-point in the Brillion zone. The calculations show that the electron-phonon coupling is driven primarily by the optical LO and TO phonon modes in graphene. The photoemission intensity from the σ band is strongly suppressed near the $\bar{\Gamma}$-point due to sublattice interference effects. These effects are removed by taking data in the neighbouring Brioullin zone. By this we have been able to disentangle the influence of sublattice interference and electron-phonon coupling. A rigorous analysis of the experimentally determined complex self-energy further supports the assignment of the observed kink to strong electron-phonon coupling and yields $\lambda \approx 0.6$, in excellent agreement with the calculations.

TT 74.7 Thu 16:30 TRE Ma

Imaging Anisotropic Carrier Dynamics in Graphene — •Sven Aeschlimann[1], Mariana Chavez-Cervantes[1], Hubertus Bromberger[1], Razvan Krause[1], Ameer Al-Temimy[2], Camilla Coletti[2], Andrea Cavalleri[1,3], and Isabella Gierz[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg, Germany — [2]Center for Nanotechnology @ NEST, Istituto Italiano di Tecnologia, Pisa, Italy — [3]Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, United Kingdom

Photo-excitation of graphene transfers electrons from the valence band to the conduction band in a direct interband transition. The initial distribution of holes and electrons is known to be anisotropic with nodes along the direction of the light polarization. We use time- and angle-resolved photoemission spectroscopy to image the initially anisotropic carrier distribution on constant energy cuts through the Dirac cone and follow its relaxation as a function of pump-probe time delay. We find that ultrafast collinear electron-electron scattering rapidly redistributes the energy among the carriers and establishes a momentum-dependent electronic temperature on time scales short compared to our experimental resolution. Momentum relaxation occurs mainly through optical phonon emission within approximately 100 femtoseconds determined from the time it takes for the electron distribution to become isotropic. Our measurements provide a complete picture of the ultrafast thermalization dynamics in photo-excited graphene.

TT 74.8 Thu 16:45 TRE Ma

Quantifying electronic band interactions in van der Waals materials using angle-resolved reflected-electron spectroscopy — •Johannes Jobst[1,2], Alexander J. H. van der Torren[1], Eugene E. Krasovskii[3], Jesse Balgley[2], Cory R. Dean[2], Rudolf M. Tromp[4,1], and Sense Jan van der Molen[1] — [1]Leiden Institute of Physics, Leiden University, The Netherlands — [2]Department of Physics, Columbia University, New York, USA — [3]Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian/Donostia, Spain — [4]IBM T.J. Watson Research Center, Yorktown Heights, USA

High electron mobility is one of graphene's key properties, exploited for applications and fundamental research alike. Highest mobility values are found in heterostructures of graphene and hexagonal boron nitride, which consequently are widely used. However, surprisingly little is known about the interaction between the electronic states of these layered systems. Rather pragmatically, it is assumed that these do not couple significantly. Here we study the unoccupied band structure of graphite, boron nitride and their heterostructures using angle- resolved reflected-electron spectroscopy. We demonstrate that graphene and boron nitride bands do not interact over a wide energy range, despite their very similar dispersions. The method we use can be generally applied to study interactions in van der Waals systems, that is, artificial stacks of layered materials. With this we can quantitatively understand the 'chemistry of layers' by which novel materials are created via electronic coupling between the layers they are composed of.

TT 74.9 Thu 17:00 TRE Ma

Magneto-optic effects of graphene at the carbon 1s edge on metallic substrates - theory and experiment — •Dominik Legut[1], Peter M. Oppeneer[2], Christine Jansing[3], Markus Gilbert[3], Andreas Gaupp[3], Hans-Christoph Mertins[3], Andrey Sokolov[4], Suk-Ho Choi[5], Hud Wahab[6], and Heiko Timmers[6] — [1]IT4Innovations Center, VSB-TU Ostrava, 17.listopadu 15, CZ 70833 Ostrava, Czech Republic — [2]Dept. of Physics and Astronomy, Box 530, S-751 21 Uppsala, Sweden — [3]FH Münster, Stegerwaldstr. 39, D-48565 Steinfurt, Germany — [4]HZB, Albert Einstein Str. 15, D-12489 Berlin, Germany — [5]Dept. of Applied Physics, Kyung Hee University, Korea — [6]Univ. of New South Wales Canberra, Australia

The optical properties at the carbon 1s of the free standing graphene utilizing the electronic structure models are calculated from first principles. For its better description the core-hole quasiparticle is taken into account. One can model it by the so-called Slater transition state employing the supercell calculation with partial hole on one of the carbon atoms with the electron charge distributed over the valence states. Another approach is to solve Bethe-Salpeter equations for the many-body electronic effects. The latter approach clearly identify the excitonic features of π- and σ-excitations of graphene. Next, optical response of the graphene on metallic substrate (Cu, Ni, and Co) is calculated and the degree of the hybridization between the p_z and d-states is determined, together with the identification of the magnetic moments. Next, using multilayerd optical code the T-MOKE and XMCD spectra are determined and compared with recently recorded data.

TT 74.10 Thu 17:15 TRE Ma

Bottom-up synthesis of graphene nanomembranes with tunable porosity — •Christof Neumann[1], Michael Mohn[2], Matthias Füser[3], David Kaiser[1], Ute Kaiser[2], Andreas Terfort[3], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm — [3]Institute of Inorganic and Analytical Chemistry, Goethe University Frankfurt, 60348 Frankfurt

The potential of 2D materials like carbon or graphene nanomembranes [1] for separation or ultrafiltration applications is based on the unique features of these novel nanomaterials having pore sizes suitable for molecular sieving and negligible thicknesses compared to the molecular mean free paths or even below. Here we present a versatile method for tuning the properties of graphene nanomembranes by conversion of 4-(1H-pyrrol-1-yl)thiophenol, 4-(2,5-dimethyl-1H-pyrrol-1-yl)thiophenol and 4-(pyrimidin-2-yl)phenylthiol self-assembled monolayers (SAMs) on polycrystalline copper foils into carbon nanomembranes (CNMs) via electron induced crosslinking and their further pyrolytic transformation into the nanoporous graphene monolayers. We characterize the resulting SAMs, CNMs and graphene-nanomembranes by different complementary techniques including X-ray photoelectron (XPS) and Raman spectroscopy, atomic force (AFM), helium ion (HIM) and high-resolution transmission electron microscopy (HRTEM) as well as by electric transport measurements. [1] A. Turchanin and A. Gölzhäuser, Adv. Mater. 28, 5075 (2016)

TT 74.11 Thu 17:30 TRE Ma

tracking electron dynamics in graphene and TMDCs — •Cephise Cacho — Artemis - Central Laser Facility, Didcot, UK

Novel quantum materials such as graphene and transition metal dichalcogenides (TMDC) are attracting vast interest particularly for their application in spintronic and optoelectronic devices. Their properties are intrinsically governed by the large momentum electrons (at the Brillouin zone K-point). In order to eject such electrons in vacuum and observe their dynamics, a high energy (>20 eV) photon source is required as well as ultrashort pulse duration. High Harmonic Generation source [1] combined to an Angle-Resolved PhotoEmission Spectroscopy (ARPES) end-station is a powerful tool to observe such electron dynamics. After an introduction on ARPES and experimental concepts, I will present an overview of recent time-resolved ARPES studies [2-6] performed at the Artemis facility.

Single-layers of MoS2, WS2 and bulk WSe2 were resonantly pumped across the band gap at the K point. Monitoring the valence/conduction bands population reveals the band dynamics during excitation. Furthermore the intervalley scattering is explored by exciting the surface with circularly polarized light.

References 1. F. Frassetto et al., Optics Express 19, 19169 (2011) 2. E. Pomarico et al., arXiv:1607.02314 (2016) 3. A. Grubišić Čabo et al., Nano Lett. 15, 5883 (2015) 4. S. Ulstrup et al., ACS Nano 10, 6315 (2016) 5. S. Ulstrup et al., arXiv:1608.06023 (2016) 6. R. Bertoni et al., arXiv:1606.03218 (2016)

TT 74.12 Thu 17:45 TRE Ma

Phase diagram of a graphene bilayer in the zero-energy Landau level — •Angelika Knothe[1,2] and Thierry Jolicoeur[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — [2]Laboratoire de Physique Théorique et Modèles Statistiques (LPTMS), Université Paris-Sud, 91405 Orsay, France

We theoretically investigate the ground state structure of bilayer graphene (BLG) in the quantum Hall regime. In BLG, the zero energy states carry, besides the real spin, two pseudospin degrees of freedom: a valley isospin and a Landau level (n = 0, n = 1) isospin. This peculiar property leads to an octet of states that is eightfold degenerate in the absence of any symmetry breaking and can be treated in the frame of quantum Hall ferromagnetism. If this SU(8) symmetry is indeed broken, an extraordinary rich phase structure emerges, with each phase characterized by a different spin and isospin configuration. Recent experiments have revealed a plethora of transitions upon variation of the strength of an applied magnetic or electric field. We start from a four-band model Hamiltonian for Bernal stacked BLG and take into account both, intrinsic symmetry breaking effects, as well as the influence of externally applied fields. Using a Hartree-Fock treatment, we study the ground state spin and isospin phases as a function of external magnetic and electric field strengths. For the different filling factors of the zero energy multiplet we predict the number of phases, as well as the nature and the properties of the respective phase transitions.

[1] Angelika Knothe and Thierry Jolicœur, arXiv:1609.04983

TT 74.13 Thu 18:00 TRE Ma

Graphene-multiferroic interfaces for spintronics applications — •Zeila Zanolli — Institute for Theoretical Solid State Physics, RWTH Aachen University and ETSF, D-52056 Aachen, Germany.

Graphene and magnetoelectric multiferroics are promising materials for spintronic devices with high performance and low energy consumption. A very long spin diffusion length and high carrier mobility make graphene attractive for spintronics. The coupling between ferroelectricity and magnetism, which characterises magnetoelectrics, opens the way towards unique device architectures. In this work[1], we combine the features of both materials by investigating the interface between graphene and $BaMnO_3$, a magnetoelectric multiferroic. We show that electron charge is transferred across the interface and magnetization is induced in the graphene sheet due to the strong interaction between C and Mn. Depending on the relative orientation of graphene and $BaMnO_3$, a quasi-half-metal or a magnetic semiconductor can be obtained. A remarkably large proximity induced spin splitting of the Dirac cones (∼300 meV) is achieved. We also show how doping with acceptors can make the high-mobility region of the electronic bands experimentally accessible. This suggests a series of possible applications in spintronics (e.g. spin filters, spin injectors) for hybrid organic-multiferroic materials and reveals hybrid organic-multiferroics as a new class of materials that may exhibit exotic phenomena such as the quantum anomalous Hall effect and a Rashba spin-orbit induced topological gap.

[1] Z. Zanolli, Scientific Reports, 6, 31346 (2016)

TT 75: Poster Session: Transport 1

Time: Thursday 15:00–19:00 Location: P2-EG

TT 75.1 Thu 15:00 P2-EG

Keldysh-FRG Approach for Inhomogeneous One-Dimensional Fermi Systems with Finite-Ranged Interactions — •Lukas Weidinger, Dennis Schimmel, and Jan von Delft — LMU München, Theresienstraße 37, München

In a previous paper (arXiv:1609.07423), we have introduced an extended coupled-ladder approximation (eCLA) scheme for 2nd-order truncated functional renormalization group (fRG) calculations in the Matsubara formalism, capable of treating finite-ranged interactions. We applied it in a static approximation and at zero temperature to models of quantum point contacts (QPCs) and quantum dots (QDs).

In this poster, we present our current follow-up work on the implementation of a dynamical eCLA within the Keldysh formalism. We pursue this for two main reasons: First, to get additional insights by obtaining real-frequency data, allowing us, for example, to compute the interacting local density of states (LDOS). This enables us also to study the finite-temperature behavior of the conductance which turned out to be unfeasible in Matsubara fRG. Second, within the Keldysh formalism we are able to study non-equilibrium effects, e.g. by applying finite source-drain voltages or temperature gradients to our systems.

TT 75.2 Thu 15:00 P2-EG

Non-equilibrium transport through a disordered molecular nanowire — Patrick Thiessen[1], Francisco Dominguez-Adame[1,2], •Rudolf A Römer[2], and Elena Diaz[1] — [1]University of Warwick, Coventry, CV4 7AL, United Kingdom — [2]Universidad Complutense, E-28040 Madrid, Spain

We investigate the non-equilibrium transport properties of a disordered molecular nanowire. The nanowire is regarded as a quasi-one-dimensional organic crystal composed of self-assembled molecules. One orbital and a single random energy are assigned to each molecule while the inter- molecular coupling does not fluctuate. Consequently, electronic states are expected to be spatially localized. We consider the regime of strong localization, namely, the localization length is smaller than the length of the molecular wire. We also take into account the electron-vibron interaction that takes place in each single molecule. We investigate the interplay between disorder and electron-vibron interaction in response to either an applied electric bias or a temperature gradient. To this end, we calculate the electric and heat currents when the nanowire is connected to leads, using the Keldysh non-equilibrium Green's function formalism. At not very high temperature, scattering by disorder dominates both charge and energy transport. We find that the electron-vibron interaction enhances the effect of the disorder on the transport properties due to the exponential suppression of tunneling.

TT 75.3 Thu 15:00 P2-EG

Implementation of transmission functions for an optimized three-terminal quantum dot heat engine — •Christian H. Schiegg, Michael Dzierzawa, and Ulrich Eckern — Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

We consider two modifications of a recently proposed three-terminal quantum dot heat engine. First, we investigate the necessity of the thermalization assumption, namely that electrons are always thermalized by inelastic processes when traveling across the cavity where the heat is supplied. Second, we analyze various arrangements of tunneling-coupled quantum dots in order to implement a transmission function that is superior to the Lorentzian transmission function of a single quantum dot. We show that the maximum power of the heat engine can be improved by about a factor of two, even for a small number of dots, by choosing an optimal structure.

TT 75.4 Thu 15:00 P2-EG

Hierarchical equations of motion approach to transport through an Anderson impurity coupled to interacting Luttinger liquid leads — •Junichi Okamoto[1,2], Ludwig Mathey[1,2], and Rainer Härtle[3] — [1]Zentrum für Optische Quantentechnologien and Institut für Laserphysik, Universität Hamburg, Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany — [3]Institut fuï Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany

We generalize the hierarchical quantum master equations (HQME) method to investigate electron transport through an Anderson impurity coupled to one-dimensional interacting leads that can be described as Luttinger liquids [1]. In comparison to noninteracting leads, Luttinger liquids involve many-body correlations and the single-particle tunneling density of states shows a power-law singularity at the chemical potential. Using the generalized HQME method, we assess the importance of the singularity and the next-to-leading order many-

body correlations. To this end, we compare numerically converged results with second and first-order results of the hybridization expansion inherent to our method. Cotunneling effects turn out to be most pronounced for attractive interactions in the leads. We also find that an interaction-induced negative differential conductance near the Coulomb blockade thresholds is suppressed compared to a first-order result. Finally, we discuss that the $n(\geq 2)$-particle correlations enter as a n-order effect and are, thus, not very pronounced at the high temperatures. [1] J. Okamoto, L. Mathey, R. Härtle, arXiv:1608.05399

TT 75.5 Thu 15:00 P2-EG

Quantifying system-bath correlations in biased quantum dot systems using the hierarchical quantum master equation technique — •Jakob Bätge and Rainer Härtle — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

We consider quantum dot systems, where system-bath correlations emerge from a continuous exchange of electrons of the dot with its environment, that is leads representing macroscopic electron reservoirs. We analyze these correlations by investigating the transient dynamics in response to time-dependent electric fields, for example a sudden change of the applied bias voltage. To this end, we use the unique properties of the hierarchical quantum master equation technique [1,2], which allow us to turn on and off system-bath correlations completely or only selected parts, at any instant of time. Thus, we are able to define measures for system-bath correlations that can be used for a systematic and quantitative analysis. Here, we present first results of such an analysis, demonstrating the use of the new measures and how they can be accessed experimentally.

[1] Jin et al., JCP 128, 234703 (2008)
[2] Härtle et al., PRB 88, 235426 (2013)

TT 75.6 Thu 15:00 P2-EG

Switching the electrical conductance of double quantum dot and quantum dot spin valve systems exploiting exchange interactions — •Sebastian Wenderoth and Rainer Härtle — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

Recently, sharp peaks in the conductance of double quantum dot and quantum dot spin valve systems have been reported [1,2,3]. Their origin has been traced back to the effect of interaction-induced renormalization [1,3] and coupling effects [2]. In this contribution, we investigate the possible use of the underlying phenomena to realize switching processes in electronic device applications by simple gate voltage operations. This includes a discussion of switching times, switching efficiencies, the underlying physical mechanisms and parameter dependencies. To this end, we employ the hierarchical quantum master equation approach, which allows us to obtain numerically converged, exact results as well as approximate results in terms of a hybridization expansion [1,3]. In particular, its time-local formulation allows us to study the switching behavior to all relevant time scales. We find that many-body interactions enhance the switching efficiency but also the switching times by an order of magnitude.

[1] Härtle et al., PRB 88, 235426 (2013)
[2] Hell et al., PRB 91, 195404 (2015)
[3] Wenderoth et al., PRB 94, 121303R (2016)

TT 75.7 Thu 15:00 P2-EG

Lab::Measurement — Measurement control and automation with Perl — Simon Reinhardt, Christian Butschkow, Alexei Iankilevitch, Alois Dirnaichner, and •Andreas K. Hüttel — Institute for Experimental and Applied Physics, Universität Regensburg, 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. A high-level layer 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 75.8 Thu 15:00 P2-EG

Unconventional superconductivity in quantum dots mediated by spin orbit coupling — •Isabel Oppenberg, Stephan Weiss, and Jürgen König — Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

We study an interacting quantum dot with two electronic levels in the presence of spin orbit (SO) interaction and a static magnetic field. The quantum dot is coupled to two normal and one superconducting lead. We integrate out the superconductor in the limit $\Delta \to \infty$. This yields an effective model for the dot with finite conventional pairing amplitude. Due to finite SO coupling together with a (noncollinear) static magnetic field, singlets and triplets are coupled and finite unconventional pairing mechanism emerge. They are described by Gorkov's Greens functions [1]. We take the coupling of the system to the normal leads into account by a realtime diagrammatic method [2]. For a symmetric and non-symmetric lead coupling case, the density matrix elements, reflecting unconventional superconducting pairing, are analyzed for different sets of parameters. Furthermore, the calculation of the nonequilibrium Andreev current and the spectrum of Andreev addition energies allows us to investigate the interplay between SO coupling and unconventional superconducting correlations on the quantum dot.

[1] Björn Sothmann, Stephan Weiss, Michele Governale and Jürgen König, PRB **90**, 220501(R) (2014)
[2] M. Governale, M.G. Pala and Jürgen König, PRB **77**, 134513 (2008)

TT 75.9 Thu 15:00 P2-EG

Utilizing SETs in single electron counting experiments — •David Reifert, Niels Ubbelohde, Ralf Dolata, Thomas Weimann, and Alexander Zorin — Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig. Germany

We fabricate dynamic quantum dots through a shallow etch process of a GaAs/AlGaAs heterostructure. These quantum dots can be operated as single electron source by periodically modulating one of the barriers of the dot. The resulting current $I = e\,f$ depends only on the pumping frequency f and the electronic charge e, which enables us to use these pumps as a new quantum current standard. We utilize superconducting aluminum single electron transistors (SETs) as ultra sensitive charge detectors to characterize the performance of such electron pumps. To increase the measurement bandwidth of our detectors we use the RF-SET technology, where we put the SET in a resonant tank circuit and measure the reflectance of this resonator. Besides increasing the bandwidth this technique enables us to multiplex several detectors. We will show the fabrication and operation of our hybrid devices consisting of semiconductor electron pumps and metallic SET detectors. Furthermore, we investigate the performance of semiconductor based SETs as charge detectors and compare them with the superconducting metallic SETs. We then utilize these devices to perform single electron counting measurement, where the electron pump act as an electron source and the SETs detects these electrons, which then will enables us to validate the precision of the pump.

TT 75.10 Thu 15:00 P2-EG

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 presented 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 and terahertz out-of plane resonances are predicted.
Europhysics Letters, 104 (2013) 27005, Phys. Rev. **B 92** (2015) 245425, errata Phys. Rev. **B 93** (2016) 239904(E), Phys. Rev. **B 92** (2015) 245426, Phys. Rev. **B 94** (2016) 165415

TT 75.11 Thu 15:00 P2-EG

Large anomalous Hall effect in the non-collinear antifer-

romagnet Mn_5Si_3 — •Christoph Sürgers[1], Thomas Wolf[2], Peter Adelmann[2], Wolfram Kittler[1], Gerda Fischer[1], and Hilbert v. Löhneysen[2] — [1]KIT, Physikalisches Institut — [2]KIT, Institut für Festkörperphysik

The anomalous Hall effect (AHE), which in long-range ordered ferromagnets appears as a voltage transverse to the current and usually is proportional to the magnetization, often is believed to be of negligible size in antiferromagnets due to their low uniform magnetization. However, recent experiments and theory have demonstrated that certain antiferromagnets with a non-collinear arrangement of magnetic moments exhibit a sizeable spontaneous AHE at zero field due to a non-vanishing Berry curvature arising from the quantum mechanical phase of the electron's wave functions. We show that antiferromagnetic Mn_5Si_3 single crystals exibit a large AHE which is strongly anisotropic and shows multiple transitions with sign changes at different magnetic fields due to field-induced rearrangements of the magnetic structure despite only tiny variations of the total magnetization. The presence of multiple non-collinear magnetic phases offers the unique possiblity to explore the details of the AHE and the sensitivity of the Hall effect on the details of the magnetic texture.

TT 75.12 Thu 15:00 P2-EG

Magnetotransport in Topological Insulator $Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}$ — •Priyamvada Bhaskar, André Dankert, Dmitrii Khokhriakov, and Saroj Dash — Chalmers University of Technology, Göteborg, Sweden

Topological insulators (TIs) provide an excellent platform to study topological quantum physics and exploring spintronic applications due to their unique gap-less spin polarized helical metallic surface states. We explore novel semiconducting TI material $Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}$ (BSTS) and report weak-anti localization (WAL) and quantum oscillations originating from surface states. Further, spin signals originating from spin-momentum locking were observed up to room temperature. From the temperature dependence of phase coherence length and the angle dependence of universal conductance fluctuations (UCF) it was inferred that the observed transport mechanisms originate from 2D, although coupling to the bulk leading to the formation of a single 2D channel cannot be ruled out. Although the angle dependence of WAL indicates surface state contribution, Shubnikov-de Haas oscillations provide for a low surface carrier concentration. However, magnetotransport in BSTS shows high spin polarization, thus showing promise as a spintronic TI. These studies provide a platform to pursue exotic physics and novel device applications predicted for TIs and its heterostructures with other 2D materials.

TT 75.13 Thu 15:00 P2-EG

Shot noise of contacts to Fe atoms and FeH_n on Au(111) — •Michael Mohr, Andreas Burtzlaff, Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel

The ballistic transport through contacts to single Fe atoms on Au(111) surfaces is investigated with a 4 K scanning tunneling microscope. The shot noise of the current is measured to obtain information about its spin polarization. The influences of other Fe atoms close to the contact and of hydrogen in the contact are addressed

TT 75.14 Thu 15:00 P2-EG

Transmission through half-metallic NiMnSb under consideration of defects and correlations — •Andreas Prinz-Zwick, Wilhelm Appelt, Liviu Chioncel, and Ulrich Eckern — Universität Augsburg

Half-metallic materials are of particular importance for achieving spin dependent transport properties for various spintronic applications. We study a (001) oriented heterostructure of epitaxial grown NiMnSb on Au and evaluate the transmission within the combined Density Functional and Non-Equilibrium Greens Function (NEGF) theory, implemented in SMEAGOL. The calculations include lattice defects such as vacancies and exchange of atoms. In addition the calculation for the clean system is compared with DFT+DMFT to quantify the influence of electronic correlations. Electronic correlations induce minority spin states in the half-metallic gap and significantly reduce the spin polarization of bulk NiMnSb. Surprisingly no significant change is seen in the transmission coefficient. These results demonstrate the localized nature of the many-body induced states in the half-metallic gap.

TT 75.15 Thu 15:00 P2-EG

Resonance phenomena in ferrocene-based single-molecule junctions — •Diana Slawig[1], Karthiga Kanthasamy[1], Markus Ring[3], Holger Butenschön[2], Christoph Tegenkamp[1], Fabian Pauly[3], and Herbert Pfnür[1] — [1]Inst. f. Festkörperphysik, Leibniz Universität Hannover — [2]Inst. f. organ. Chemie, Leibniz Universität Hannover — [3]FB Physik, Universität Konstanz

Ferrocene dithiol (FDT) molecules as molecular junctions and switches are particularly attractive because of their high conductance and their rotational flexibility. In our study of electrical transport through single FDT molecules between Au contacts via the break junction technique it turns out that the conductance depends strongly on the chemical end groups. This dependence allows tuning of the energy level alignment of HOMO and LUMO relative to the Fermi energy of the electrodes, as demonstrated by the comparison between ferrocene-1, 1′-diamine (FDA) and FDT, making FDT a much better conductor than FDA. Comparison of the experimental results with DFT calculations based on the single level model suggest changes of binding geometries of the molecule at the electrodes as a function of electrode separation for both molecules. Particularly interesting are resonances in the IV-curves of FDT at fixed contact distances in the conductance range (at zero bias) between $0.1\,G_0$ to $0.56\,G_0$. This phenomenon can be described by the Fano resonance model, as verified for selected molecular binding geometries in DFT simulations, which, however yields a too high temperature dependence. Therefore, further possible contributions from inelastic transport processes will also be discussed.

TT 75.16 Thu 15:00 P2-EG

Constructing nanoelectronic circuits by top-down and bottom-up strategies — •Filip Kilibarda, Torsten Sendler, Dipjyoti Deb, Muhammad Bilal Khan, Bezu Teschome, and Artur Erbe — Helmholtz - Zentrum Dresden - Rossendorf, Dresden, Germany

The construction of nanoelectronic circuits requires the development of bottom-up strategies, which can be combined with top-down structuring. We show how reconfigurable silicon nanowires are produced using electron-beam lithography and reactive ion etching. Such structures can be used as large-scale electrodes to networks of self-assembled electronics on the nanoscale. As a first step towards the development of nanoscale circuits by self-organization, we demonstrate the construction of nanoscale metallic wires based on metallized DNA origamis. Active building blocks with smallest dimensions on the molecular scale are developed in single molecule contacts. The properties of those junctions need to be characterized. We have demonstrated that the mechanically controllable break junction (MCBJ) technique can be successfully used to determine the properties of electronic transport through single organic molecules and that the participating molecular energy levels and the metal-molecule coupling can be characterized using this technique. Further developments are based on the use of more complex molecules, which can, for example, be used as single molecule switches. We present the first demonstration of a single molecule junction, in which the molecule is switched in situ from the non-conducting off-state to the conducting on-state.

TT 75.17 Thu 15:00 P2-EG

Design rules for molecular electronics: Theoretical and experimental approach — Lokamani Lokamani[1], •Filip Kilibarda[1], Jannic Wolf[2], Peter Zahn[1], Thomas Huhn[2], Sibylle Gemming[1,3], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, 01314 Dresden, Germany — [2]Universität Konstanz, 78457 Konstanz, Germany — [3]Institute of Physics, Technische Universität, 09107 Chemnitz, Germany

Diarylethenes, a class of photosensitive molecules which exhibit photochoromism, can be switched between open- and closed-ring isomers. In break-junction experiments diarylethene derivatives in open and closed-ring forms can be distinguished by a low and high conductance state respectively with a difference in current levels of about one order of magnitude.

Here, we explore the underlying design rules for modulating electronic transport in derivatives of diarylethene. In particular, we analyze the effect on molecular orbitals due to various electron accepting and donating groups and in turn the modulation of the conductance properties of single molecules attached to gold electrodes.

We have demonstrated that the mechanically controllable break junction (MCBJ) technique can be used to classify and determine the properties of electronic transport through single organic molecules. We present an outlook on experimental methods for exploring the underlying design rules for diarylethene molecules and derivatives. As a result,

we show how the addition of different side groups modifies electronic behavior of the molecules.

TT 75.18 Thu 15:00 P2-EG

Ab-initio Simulation of Quantum Transport through Silane Molecular Wires — •María Camarasa-Gómez[1], Haixing Li[2], Daniel Hernangómez-Pérez[1], Latha Venkataraman[2], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, D-93050 Regensburg, Germany — [2]Department of Applied Physics and Applied Mathematics, Columbia University, New York, New York 10027, United States

The transport properties of molecular wires are sensitive to the relative alignment of the energies of the molecular orbitals and the Fermi-energy of the contact electrodes. A natural expectation is that the alignment shifts when one contact material, e.g., Au is replaced by another material, e.g., Ag; to lowest order, the shift should reflect the difference in the work functions [1]. We have performed an elaborate set of ab-initio transport calculations that puts this hypothesis to a test.

Motivated by recent experiments, we adopt a silane molecular wire as a paradigm system. We calculate the transmission function for Au and Ag substrates, for thiol- and amino- anchor groups [2] and a variety of different contact geometries. While our results qualitatively confirm the original hypothesis, we also observe other electrode related mechanisms that appear to be of similar magnitude compared to the work function shift. Our theoretical analysis will be compared to experimental data.

[1] T. Kim et al., NanoLett. 13, 3358 (2013)
[2] Y. Kim et al., ACS Nano 5, 4104 (2011)

TT 75.19 Thu 15:00 P2-EG

Vibrational excitations in current-driven single-molecule junctions — •Joachim Reichert[1], Hai Bi[1], Carlos-Andres Palma[1], Yuxiang Gong[1], Mark Elbing[2], Marcel Mayor[2,3], and Johannes V. Barth[1] — [1]Physik-Department, Technische Universität München, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Department of Chemistry, University of Basel, Switzerland

In order to advance the development of unimolecular electronic devices, it is mandatory to improve understanding of electron transport and its loss mechanisms in single molecules. One fundamental challenge in molecular electronics is the quantitative determination of charge-vibrational coupling for well-defined single-molecule junctions.

Here we determine the charge-vibrational coupling for a current-carrying, chemically defined metal-molecule-metal junction by synchronous vibrational and current-voltage spectroscopy. Measuring the steady-state vibrational distribution during charge transport in a bis-phenylethynyl-anthracene derivative by Raman scattering allows us to quantify the charge-vibrational coupling constant in this single-molecule system. Our work provides means to directly measure inelastic losses in (macro)molecular circuitry and introduces a general technique to perform optical spectroscopy on single-molecule junctions.

TT 75.20 Thu 15:00 P2-EG

Large magnetoresistance in single radical molecular junctions — •Sebastian Hambsch[1], Ryoma Hayakawa[1,2], Amin Karimi[1], Jannic Wolf[1], Thomas Huhn[1], Martin Sebastian Zöllner[3], Carmen Herrmann[3] und Elke Scheer[1] — [1]University of Konstanz, 78457 Konstanz — [2]NIMS, Tsukuba 305-0044, Japan — [3]University of Hamburg, 20146 Hamburg

We present the charge transport properties of single radical molecule junctions formed by a break junction technique at 4.2 K in magnetic field B. In this study, stable and neutral radical molecules based on an oligo(p-phenylene ethynylene) (OPE) backbone (TEMPO-OPE) were placed on a freestanding gold (Au) bridge. We observe large positive magnetoresistance (MR) up to 287 % at 4T from TEMPO-OPE molecules when B was applied perpendicular to the sample plane [R. Hayakawa et al. Nano Lett. 16, 4960 (2016)]. The averaged MR was one order of magnitude larger than that of the analogous non-radical OPE molecule. The analysis of the MR, of IVs and of inelastic electron tunneling spectra reveal an effective reduction of the electronic coupling between the current-carrying molecular orbital and the electrodes with increasing B. Our findings thus provide a new physical approach for tuning the charge transport via radical molecules.

TT 75.21 Thu 15:00 P2-EG

Beyond the Born-Oppenheimer approximation: Non-adiabatic processes in manganites — •Michael ten Brink[1], Peter E. Blöchl[2], Stephanie Mildner[3], and Christian Jooss[3] — [1]Institute for Theoretical Physics, University of Goettingen — [2]Institute for Theoretical Physics, Clausthal University of Technology — [3]Institute for Materials Physics, University of Goettingen

Non-adiabatic processes in the combined atomic and electronic dynamics are explored using two simple model systems, the Holstein model and the Jahn-Teller model. Numerically exact simulations demonstrate processes for the optical excitation and the subsequent relaxation into the ground state. The Holstein model is the classical model for polarons and its dimer allows to demonstrate the role of electronic and structural transitions in an optical excitation. We demonstrate (1) predominantly electronic interband excitations, which are Frank-Condon like, (2) predominantly structural intra-band transitions related to tunnel processes, and (3) an electronic transition that critically depends on the presence of thermal phonons. The latter gives rise to a distinct absorption band with strong temperature dependence. The dominant relaxation mechanisms lead through conical intersections, for which the Jahn-Teller model is the classical model system. We present the transition of a quantum mechanical, nuclear-electronic wave packet through the conical intersection. We discuss the results of measured optical absorption spectra in manganites in view of our theoretical findings.

This work is supported by the Deutsche Forschungsgemeinschaft via SFB 1073 through projects B03 and C03.

TT 75.22 Thu 15:00 P2-EG

Comparison of dephasing models for molecular wires — •Patrick Karasch[1], Verena Gupta[1], Gabriele Penazzi[1], Alessandro Pecchia[2], Dmitry A. Ryndyk[1], and Thomas Frauenheim[1] — [1]Bremen Center for Computational Materials Science, Universität Bremen, Germany — [2]CNR-ISMN, Roma, Italy

In this work, we investigate the decoherence effects which play an important role in the charge transport characteristics of quantum wires at room temperature. For molecular junctions and onedimensional molecular wires we investigate the distinct dephasing models to calculate and compare the effective resistances and investigate the crossover from coherent Landauer transport to ohmic behavior in long wires. First, we consider the Momentum Relaxing Dephasing (MRD) and the Büttiker Probe (BP) models. These approaches rely on the empirical coupling strength of electronic states to the environment. Then we introduce the electron-phonon dephasing model and consider different approximations including the first Born approximation (BA) and the self-consistent Born approximation (SCBA). Besides, we consider the interplay of disorder and dissipation. Our theoretical method is based on the nonequilibrium Green function approach to quantum transport. To go towards the atomistic ab initio theory, we implemented the method in combination with the density functional based tight binding (DFTB) theory [1] within the DFTB+ code and DFTB-NEGF transport method.

[1] G. Penazzi et al., J. Phys. Chem. C **120**, 16383 (2016)

TT 75.23 Thu 15:00 P2-EG

Parallel fabrication of an entire array of carbon nanotubes devices: a new approach to stamping techniques — •Christian Bäuml, Korbinian Mühlberger, Julian Heger, Christoph Strunk, and Nicola Paradiso — University of Regensburg

We present a new approach to the fabrication of devices based on carbon nanotubes (CNTs) in the low disorder regime. Our fabrication method consists of growing CNTs on a transparent quartz chip and stamping them on an array of tens of devices. The quartz chip and the recipient chip are designed in such a way that during the stamping process the CNTs do not touch any substrate and stays suspended on the electrodes of the recipient devices. The parallel transfer of tens of CNTs highly increases the average number of usable devices per chip. The resulting CNT-based devices are characterized via transport measurements at different temperatures down to the mK-regime. The separation of growth chip from the measurement chip allows one to freely choose the material for the electrodes, opening the way for the implementation of CNT-based devices with superconducting or ferromagnetic leads.

TT 75.24 Thu 15:00 P2-EG

Shot noise measurements on an ultra clean CNT quantum dot — •Michael Schafberger, Daniel Steininger, Nicola Paradiso, and Christoph Strunk — University of Regensburg

Shot noise measurements are a fundamental tool for studying the correlation between charge carriers in mesoscopic devices. Here we present simultaneous measurements of shot noise and conductance on an ultra clean carbon nanotube (CNT) quantum dot. In order to favor defect free and unperturbed CNTs, chemical vapor deposition growth is performed as last nanofabrication step on to Pt-contacts. The sample shows a four-fold symmetry in the Coulomb oscillations. Boson-like excitation lines are observed in certain gate-voltage ranges. We investigate the shot noise on the electron-side, as well as the hole-side of the carbon nanotube and discuss the results.

TT 75.25 Thu 15:00 P2-EG

Magnetic field control of the electron-vibron coupling in a carbon nanotube quantum dot — Peter L. Stiller, Daniel R. Schmid, Christoph Strunk, and •Andreas K. Hüttel — Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

Quantum dots defined in suspended single wall carbon nanotubes define a prototypical nano-electromechanical system: the quantized harmonic oscillator behaviour of the longitudinal vibration mode becomes clearly visible in low-temperature transport spectroscopy.

Here, we present measurements on a nanotube device tuned to the region of $0 \leq N \leq 2$ trapped electrons, i.e., close to the electronic band gap. A highly localized electronic system in strong Coulomb blockade is present. At finite bias, we demonstrate the emergence of Franck-Condon sidebands in single electron tunneling, corresponding to the longitudinal vibration, solely in a magnetic field along the carbon nanotube axis.

The magnetic field evolution of the Franck-Condon coupling factor g is analyzed. For the two-electron ground state it increases from $g = 0$ starting at $B \simeq 1.5\,\mathrm{T}$ and saturates around $B \simeq 3.3\,\mathrm{T}$, however, for different electronic quantum states differing vibronic side band behaviour is found.

We present tentative models, based on the influence of axial magnetic fields on the localization of the electronic wave function. The impact of spin/valley quantum numbers on the electron-vibron coupling is discussed.

TT 75.26 Thu 15:00 P2-EG

Determining the carbon nanotube chiral angle from electronic Fabry-Perot interference — Alois Dirnaichner[1,2], Miriam del Valle[2], Karl Götz[1], Felix Schupp[1], Nicola Paradiso[1], Milena Grifoni[2], Christoph Strunk[1], and •Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany — [2]Institute for Theoretical Physics, Universität Regensburg, Regensburg, Germany

Connecting low-temperature transport spectroscopy features with a specific microscopic nanotube structure has been an elusive goal so far. While in Coulomb blockade many aspects of the discrete level spectrum are well-understood, a closer look leads to fascinating (and puzzling) hard questions. Here, we apply a complementary approach and analyze the Fabry-Perot interference pattern of a carbon nanotube strongly coupled to metallic leads. By tuning a gate voltage over a large range, the trigonal warping of the Dirac cones can be probed. This, in combination with the valley degree of freedom, leads to a superstructure in the interference pattern, i.e., a secondary interference.

Measurements on an ultraclean, long and suspended carbon nanotube device at millikelvin temperatures are complemented with tight binding calculations of the transmission for specific chiralities and analytic modelling. Taking symmetry classes of nanotubes, but also effects of symmetry breaking at the contacts into account, we show that the crucial parameter for the robust secondary interference pattern is the chiral angle. Consequently, the pattern provides valuable information for determining the structure of a carbon nanotube device.

TT 75.27 Thu 15:00 P2-EG

Towards GHz reflection on a suspended carbon nanotube — Pascal Brunner, •Stefan Blien, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

Applying GHz signals as bias of a single electron tunneling device, as, e.g., a carbon nanotube, poses an obvious challenge. The impedance mismatch of typical radiofrequency electronics at $Z_0 = 50\,\Omega$ and a quantum conductor at $Z_L \gg 6\,\mathrm{k}\Omega$ leads to predominant signal reflection. This effect can be avoided by using an impedance matching network. A specific circuit which has already been successfully used to that purpose in literature is the so-called stub tuner.

We present low-temperature reflection measurements on stub tuner geometries intended for the in-situ growth of "ultraclean" carbon nanotubes as loads. The utilized superconductor is a rhenium-molybdenum alloy highly resistant to the nanotube growth process. For a load resistance of $Z_L = 50\,\mathrm{k}\Omega$ impedance matching is demonstrated with a return loss $> 70\,\mathrm{dB}$. The stub tuner properties are consistent with previous material characterization. Finally we discuss fabrication challenges for devices integrating in-situ grown carbon nanotubes.

TT 75.28 Thu 15:00 P2-EG

Current flow paths in deformed graphene and carbon nanotubes — Erik Kleinherbers, •Nikodem Szpak, and Ralf Schützhold — Faculty of Physics, University of Duisburg-Essen, Germany

Due to imminent applications in nanoelectronics it is of high interest to understand the precise conductance properties of deformed graphene and bent carbon nanotubes. Since low-energy electronic excitations behave like massless Dirac fermions the current flow can be approximated semiclassically and used as a guide in the design of conducting nanoelectronic elements and nanosenors. Taking into account the curvature effects as well as an emerging inhomogeneous pseudo-magnetic field we calculate the current flow paths theoretically and compare them with numerical simulations of the full electronic transport.

TT 75.29 Thu 15:00 P2-EG

Coherent exciton transport in double-bilayer graphene — •Bogusz Bujnowski[1], Dario Bercioux[1,2], Jerôme Cayssol[3], and Sebastian Bergeret[1,4] — [1]Donostia International Physics Center (DIPC) - Manuel de Lardizabal 5, E-20018 San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation for Science, Maria Diaz de Haro 3, 48013 Bilbao, Spain — [3]LOMA (UMR-5798), CNRS and Université Bordeaux - F-33045 Talence, France — [4]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU E-20018 Donostia-San Sebastián, Basque Country, Spain

We study exciton condensate formation and coherent transport in a system of two graphene bilayers that are separated by hexagonal boron-nitride. A variety of excitonic-phases has been identified by varying separately the carrier density in the graphene sheets of each bilayer as well as the distance between the bilayer sheets [1]. The richness of the phase diagram could be the key to understand the interesting transport properties observed in recent experiments [2,3]. We aim to explain some key experimental features in terms of peculiar transport properties associated to excitonic condensates [4].

[1] J. Su and A.H. MacDonald, arXiv:1611.06410 (2016).
[2] J.I.A. Li *et al.*, Phys. Rev. Lett., **117** 046802 (2016).
[3] K. Lee *et al.*, Phys. Rev. Lett. **117**, 046803 (2016).
[4] M. Rontani & L. J. Sham, Phys. Rev. Lett. **94**, 186404 (2005).

TT 75.30 Thu 15:00 P2-EG

Spin and Charge Transport in Tailored Carbon Allotropes such as Doped Graphene — •Marie-Luise Braatz[1,2], Nils Richter[1,2], Hai I. Wang[1], Axel Binder[3], Mischa Bonn[4], and Mathias Klăui[1,2] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz (MAINZ), 55128 Mainz, Germany — [3]BASF SE, 67056 Ludwigshafen, Germany — [4]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

Graphene exhibits extraordinary properties, however, pristine graphene does not show a band gap as needed for many applications. One of the routes to change that is chemical doping [1]. Here we investigate the effect of heteroatom-dopants on the structure and on the electronic and magnetic properties of graphene. The growth conditions are systematically varied to achieve different dopant concentrations. The resulting structural properties are characterized by Raman and electron microscopy while the charge transport is probed by THz spectroscopy. To correlate the structure and charge properties with magnetotransport we determine the magnetoresistance as a function of temperature and field [2].

[1] H. Wang et al., ACS Catal. 2, 781 (2012)
[2] M. Rein et al., ACS Nano 9, 1360 (2015)

TT 75.31 Thu 15:00 P2-EG

THz Magnetooptical Conductivity in epitaxially grown Graphene Samples — •Markus Göthlich[1], Cay-Christian Kalmbach[2], Mattias Kruskopf[2], Klaus Pierz[2], Franz-Josef Ahlers[2], and Andreas Hangleiter[1] — [1]Institut für Angewandte

Physik, Technische Universität Braunschweig, Mendelssohnstraße 2, D-38106 Braunschweig — [2]Physikalisch Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig

Graphene – first isolated in 2004 – has a remarkable Landau quantization given by $E_L = \mathrm{sgn}(n)\sqrt{\Delta^2 + 2\hbar v_F^2 e|Bn|}$ with Landau-level index n and band gap 2Δ (if one is opened). This leads to a strong separation of Landau-levels of low indices even at low magnetic fields. This strong Landau-level separation can be used for the detection of radiation in the THz spectral range by cyclotron resonance as shown theoretically in Phys. Stat. Sol. C **8**, 1208 (2011). In this contribution we are investigating the conductivity of graphene in the case of cyclotron resonance absorption in the THz spectral range. The carrier concentration of the device can be tuned by photo chemical gating. The samples are first characterised by Shubnicov-da Haas-measurements. Then, our photoresponse measurements are done in a cryostat at 4 K, in a magnetic field tunable up to 10 T and with a pGe-Laser with a tunable emission wavelength in the range of 120–180 μm corresponding to $\hbar\omega_{\mathrm{photon}} \approx 10$ meV. Our aim is a photodetector device based on epitaxial graphene on Si-face SiC that is responsive and spectrally selective and that can be used at elevated temperatures and low magnetic fields.

TT 75.32 Thu 15:00 P2-EG

Simulation of Electron Transport through Graphene-Molecule Junctions — •Dominik Weckbecker[1], Susanne Leitherer[1], Konrad Ullmann[2], Pedro B. Coto[1], Heiko B. Weber[2], and Michael Thoss[1] — [1]Institute for Theoretical Physics and Interdisciplinary Center for Molecular Materials, University Erlangen-Nürnberg — [2]Chair of Applied Physics and Interdisciplinary Center for Molecular Materials, University Erlangen-Nürnberg

While most experiments on single-molecule junctions have employed metal electrodes, recent works demonstrate that graphene has a number of advantages over metallic leads [1-2]. In this contribution, we investigate charge transport in graphene-molecule junctions employing a theoretical approach that combines first-principles electronic structure methods with nonequilibrium Green's function transport theory. Specifically, we consider zigzag and armchair graphene terminated leads and two molecule-lead coupling regimes: (i) strong coupling with covalent binding and (ii) weak coupling, in which the molecular bridge is anchored to the leads by weak bonding interactions. We analyze how the different termination of the graphene electrodes and the molecule-lead coupling affects the transport characteristics [3]. The effect of the structure of the molecular bridge on the conductance properties of the junctions is also discussed [1].

[1] K. Ullmann et al., Nano Lett. 15, 3512 (2015)
[2] C. Jia et al., Science 352, 1443 (2016)
[3] I. Pshenichnyuk et al., J. Phys. Chem. Lett. 5, 809, (2013)

TT 76: Poster Session: Transport 2

Time: Thursday 15:00–19:00 Location: P2-OG1

TT 76.1 Thu 15:00 P2-OG1

Vibrational lasing in a nanomechanical resonator by spin-polarized current — •Mattia Mantovani[1], Andrew Armour[2], Wolfgang Belzig[1], and Gianluca Rastelli[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]School of Physics and Astronomy, University of Nottingham, NG7 2RD Nottingham, United Kingdom

We study the nonequilibrium dynamics of a nanomechanical resonator, realized by a suspended carbon nanotube quantum dot in contact with two ferromagnetic leads, in which the dot's spin is coupled to the vibrational flexural modes [1, 2]. We show that, for an appropriate configuration of the two dot's spin levels and orientation of the magnetization in the leads, the system encodes a single-atom laser [3] where the mechanical vibration plays the role of the cavity, with frequency equal to the Zeeman splitting of the two levels. Moreover, such a system has unique features, as one can not neglect the effects of: (i) finite temperature for such low-frequency resonators ($<$ 100 MHz) and (ii) the nonlinear forces for strong, amplified amplitudes of oscillation. To understand how these effects modify the physics of the single-atom laser, we solve numerically the associated Lindblad equation to compute the average phonon occupation, the Fano factor and the spin-polarized current as a function of the bias voltage and other parameters. We show that the lasing threshold is within the experimental range for magnetic polarization and spin-vibration coupling strength.

[1] P. Stadler et al., PRL 113, 047201 (2014); PRB 91, 085432 (2015)
[2] A. Pályi et al., PRL 108, 206811 (2012)
[3] Y. Mu, M. Savage, PRA 46, 5944 (1992).

TT 76.2 Thu 15:00 P2-OG1

Violation of the Cauchy-Schwarz inequality in two microwave cavities coupled to two parallel quantum dots — •Felicitas Hellbach, Fabian Pauly, Wolfgang Belzig, and Gianluca Rastelli — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

Since the realization of high quality superconducting microwave cavities [1], the so-called "circuit quantum electrodynamics" enables the possibility to investigate the coherent interaction of light and matter. Artificial atoms can be realized with quantum dots, and experiments have already proved strong coupling between a quantum dot and a microwave cavity [2]. We study two parallel quantum dots arranged in the geometry of an Aharonov-Bohm interferometer (ABI) [3]. Each dot is capacitively coupled to a microwave cavity. We explore how quantum correlation and entanglement between the two cavity fields is generated by the coherent transport of a single electron traveling in two different paths of the ABI. We calculate the second-order coherence function by use of a diagrammatic perturbative expansion (Keldysh Green's functions) to the fourth order in the dot-cavity coupling constant, taking into account vertex corrections. Ultimately, we test the Cauchy-Schwarz inequality for varying magnetic flux.

[1] A. Wallraff et al., Nature 431, 162 (2004)
[2] M. R. Delbecq et al., Nat. Commun. 4, 1400 (2013)
[3] A. W. Holleitner et al., Phys. Rev. Lett. 87, 256802 (2001)

TT 76.3 Thu 15:00 P2-OG1

Entanglement in propagating two-mode squeezed microwave states — •B. Ghaffari[1,2], K. G. Fedorov[1,2], S. Pogorzalek[1,2], P. Yard[1,2], P. Eder[1,2,3], M. Fischer[1,2,3], J. Goetz[1,2], E. Xie[1,2,3], A. Marx[1], F. Deppe[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

Josephson parametric amplifiers (JPAs) can be employed for the generation of itinerant quantum signals in the form of propagating two-mode squeezed states (TMSSs), which are essential for quantum communication protocols. Further applications of TMSSs include quantum information processing with continuous variables, or novel ideas of building quantum annealing networks based on JPAs. All these fields make use of multiple JPAs for entanglement generation and manipulation, and therefore require detailed knowledge of their physical properties. In our experiments, we employ two flux-driven JPAs at the inputs of an entangling hybrid ring in order to generate two-mode squeezing between the hybrid ring outputs. We perform tomography of the resulting TMSSs and experimentally investigate the robustness of the entanglement to noise and finite-time delays.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria, and the IMPRS 'Quantum Science and Technology'.

TT 76.4 Thu 15:00 P2-OG1

Noise spectroscopy by dynamical decoupling of a transmon qubit — •Tim Wolz, Andre Schneider, Jochen Braumüller, Martin Weides, and Alexey V. Ustinov — Institute of Physics, Karlsruhe Institute of Technology, Germany

Superconducting qubits are promising candidates as elements of quantum computers. Environmental noise limits coherence times of superconducting qubits. Improving coherence times requires a detailed knowledge about noise mechanisms. To obtain the noise power spectral density (PSD) of a qubit system, dynamical decoupling pulse sequences can be employed. Such sequences comprise several gates to

refocus dephased qubits and effectively act as frequency filters. Hence, by knowing the properties of the frequency filter and measuring the qubit's state, the noise PSD can be scanned, as it was already shown for a flux qubit [1]. In this work, noise spectroscopy is performed on a tunable concentric transmon qubit [2] by using dynamical decoupling. Because of the low anharmonicity of the transmon, gate errors play a severe role in distorting the qubit's state and subsequently the noise PSD. By using DRAG [3] pulses, we are able to accomplish sufficiently precise gates, and can thus confidently extract the noise PSD. Another advantage of this method is its universality, i.e., no functional form of the PSD needs to be assumed, and hence it can also be applied to environmental magnetic field sensing.

[1] J. Bylander et al., Nature Phys. 7, 565 (2011)
[2] J. Braumueller et al., Appl. Phys. Lett. 108, 032601 (2016)
[3] F. Motzoi et al., Phys. Rev. Lett. 103,110501 (2009)

TT 76.5 Thu 15:00 P2-OG1

Superconducting microwave resonator designs for electron paramagnetic resonance at millikelvin temperatures — •Petio Natzkin[1,2], Stefan Weichselbaumer[1,2], Christoph W. Zollitsch[1,2], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Nanosystems Initiative Munich, Munich, Germany

Superconducting coplanar microwave resonators are used in a large variety of applications, ranging from radiation detectors to experiments in quantum information processing. We use superconducting microwave resonators made from Niobium for electron paramagnetic resonance spectroscopy at millikelvin temperatures. The coplanar lumped-element design garanatees small mode volumes and large filling factors. Together with the high quality factor in the order of 10^4, this results in an increased spin sensitivity compared to conventional EPR resonators. However, the field distribution of such a quasi two-dimensional resonator is typically inhomogeneous hindering a coherent manipulation of the spin ensemble. We present the investigation of different resonator designs with particular emphasis on the homogeneity of the B_1 field. Furthermore, we compare the predictions of simple analytical models and finite element simulations with first characterization measurements of these resonator types.

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TT 76.6 Thu 15:00 P2-OG1

Time-Translation Symmetry Breaking and First-Order Phase Transitions in Periodically Driven Quantum Oscillators — Jennifer Gosner[1], •Björn Kubala[1], Mark Dykman[2], and Joachim Ankerhold[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany — [2]Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan, USA

Periodically driven damped nonlinear oscillators show under sufficiently strong driving (dynamical) bifurcations. Typically the driving is given by frequencies close to the eigenfrequency of the system or twice the eigenfrequency. Here we analyze the general situation with a drive close to the Mth overtone. We provide the relation between eigenstates in the frame rotating with the oscillator's eigenfrequency and standard M-period Floquet states, discuss time-translational symmetry breaking, and develop a detailed analysis of the phase-space structure and its symmetries.

General results are then illustrated for driving close to three times the eigenfrequency. We find that, in the presence of dissipation, a quantum oscillator can support three states of period-three vibrations that co-exist with the state of no vibrations. With varying detuning a first-order transition appears, where the populations of these states change exponentially strongly. We study the rates of switching between the stable states and their peculiar scaling behavior near bifurcation points. The results allow revealing "time crystals" in simple quantum systems, including the systems studied in circuit QED.

TT 76.7 Thu 15:00 P2-OG1

Dynamics of the pulsed central spin model and the validity of the rotating wave approximation for short pulses — •Lars B. Gravert and Götz S. Uhrig — Lehrstuhl für theoretische Physik I, Technische Universität Dortmund, Germany

We analyze the effect of different pulses and sequences to the *central spin model* (CSM), especially the influence of the pulse duration and the sequence duration. We compare different setups for the couplings between the central spin and the spin bath as well as for the couplings between bath spins. These setups address experimental systems, e. g. electron spins in quantum dots or ^{13}C in adamantane.

By utilizing the *density matrix renormalization group* (DMRG) we are able to treat larger spin baths than most other numerical approaches while retaining a full quantum mechanical description. In addition we can choose the couplings between the spin bath and the central spin arbitrarily. We employ an analytic solution for homogeneous couplings, i. e. all bath spins are coupled equally to the central spin. Small spin baths will be approached by standard techniques, e. g. *exact diagonalization* (ED).

In addition we analyze the validity of the *rotating wave approximation* (RWA) regarding composite pulses with fast alternating pulse amplitudes. For these pulses additional errors occur within the RWA due to the assumed sharp edges between the different pulse amplitudes. This error is decreased for finite rise times of the pulse amplitudes as well as for high external magnetic fields.

TT 76.8 Thu 15:00 P2-OG1

Strain Engineering of the Band Structure of HgTe Quantum Wells — •Lukas Lunczer, Philipp Leubner, Christoph Brüne, Hartmut Buhmann, and Laurens W. Molenkamp — Experimentelle Physik III, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The HgTe quantum well (QW) is a well-characterized two-dimensional topological insulator (2D TI). Its band gap E_G is relatively small (typically in the order of 10 meV), which restricts the observation of purely topological conductance to low temperatures.

Here, we utilize the strain dependence of the band structure of HgTe QWs to address this limitation. We use CdTe-$Cd_{0.5}Zn_{0.5}$Te strained-layer superlattices (SLS) on GaAs as virtual substrates with adjustable lattice constant to control the strain of the QW.

We present magnetotransport measurements, which demonstrate a transition from a semimetallic to a 2D-TI regime in wide QWs, when the strain is changed from tensile to compressive.

Most notable, we demonstrate a much enhanced energy gap of 55 meV in heavily compressively strained QWs. This value exceeds the highest possible gap on common II-VI substrates by a factor of 2-3, and extends the regime where topological conductance prevails to much higher temperatures.

TT 76.9 Thu 15:00 P2-OG1

Separate influencing of the top and bottom surface states in the three dimensional topological insulator HgTe — •Fabian Schmitt, David Mahler, Cornelius Thienel, Kalle Bendias, Christoph Brüne, Harmut Buhmann, and Laurens Molenkamp — Physikalisches Institut, Lehrstuhl für Experimentelle Physik 3, 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 a tensile strain induced band gap opening [1]. The magneto transport data indicates transport dominated by the two surfaces perpendicular to the magnetic field. This dominance was observed over a wide density range by the use of an Au top gate, which influences the two surfaces simultaneously and has been explained by the Dirac-screening of the surface states [2]. Now we demonstrate that the introduction of an additional back gate created by epitaxial growth on an n-doped GaAs substrate allows us to change the occupation of the top and bottom surface states individually. This can be exhibit by transport measurements at low temperatures and high magnetic fields.

TT 76.10 Thu 15:00 P2-OG1

A new wet etching method and a low-temperature gate process for fabrication of high-quality HgTe microstructures — Kalle Bendias, •Valentin Müller, Pragya Shekhar, Saquib Shamim, Hartmut Buhmann, and Laurens W. Molenkamp — EP3, Physikalisches Institut, Universität Würzburg

In recent years, HgTe has attracted much interest within basic semiconductor research due to its inverted band structure, which gives rise to intriguing topological properties. Despite the extensive research effort spent on HgTe, fabrication of microstructures still poses considerable challenges to the experimenter. The main reasons are the high volatility and reactivity of Hg, which ask for low-temperature lithography processes in combination with very specific chemicals.

Here we show recent improvements in the lithography process for

gateable micro- and macrostructures. For fabrication of devices, we now use a new wet etch method in combination with a low temperature, self-aligned ALD gate process.

The high performance of the developed process is demonstrated with microscopic HgTe quantum well Hall bars, which reliably show QSHE edge channel transport. Additional measurements on macroscopic Hall bars allow for a comparison with previously used gate stacks.

TT 76.11 Thu 15:00 P2-OG1

Ohmic Contacts on HgTe Quantum wells - a SEM study — •Simon Hartinger, Johannes Kleinlein, Hartmut Buhmann, and Laurens W. Molenkamp — EP3, Physikalisches Institut, Universität Würzburg

In HgTe/CdTe quantum wells above a critical thickness one can observe the topological nature of these heterostructures, called Quantum Spin Hall Effect and, in addition, the quantum Hall effect in high magnetic fields. One crucial part to observe the QSHE and the QHE is the microscopic nature of the contact material, which, for example, can cause contact problems in high magnetic fields. In this work we focus on the interface between ohmic contacts and HgTe/CdTe based quantum wells. We show SEM images of HgTe quantum wells cross sections with different contacts prepared by Focused Ion Beam milling, to analyze the intermixing of the contact material and the Quantum Well heterostructure.

TT 76.12 Thu 15:00 P2-OG1

Topological semimetals and insulators in three-dimensional honeycomb materials — •Dennis Wawrzik, David Lindner, Maria Hermanns, and Simon Trebst — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

In Fermi liquid theory, conventional metals are described via their (d-1)-dimensional Fermi surface for an electronic lattice structure in d spatial dimensions. With the discovery of Dirac matter, most prominently in graphene and on the surfaces of topological insulators, semimetals have become the subject of intense research efforts. In these semimetals, conduction and valence bands touch only at a discrete set of points or along nodal lines (for three-dimensional structures). Here we discuss a family of three-dimensional honeycomb structures that exhibit a variety of topological (semi)metals with Weyl nodes, Dirac nodal lines or flat bands arising already in simple electronic tight-binding models. In the presence of spin-orbit coupling some of these structures give rise to topological insulators. Our classification of these states can be understood from an elementary symmetry analysis of the underlying lattice structures.

TT 76.13 Thu 15:00 P2-OG1

Computing topological invariants in two-dimensional periodically driven systems — •Bastian Höckendorf, Andreas Alvermann, and Holger Fehske — Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, Greifswald, Germany

Periodically driven systems feature topological phenomena that have no analog for systems in equilibrium. Various topological invariants have been proposed to classify these phenomena but they are in general not easily computable. We show that these invariants can be connected to degeneracies of the time- and momentum-dependent spectrum of the time-evolution operator. By assigning a Chern number - a quantity that is numerically easily accessible - to each degeneracy and expressing the invariants as functions of these Chern numbers we can calculate the different invariants using one unifying concept. We demonstrate this approach for driven Harper, Kane-Mele and graphene models which are representatives of two-dimensional periodically driven systems with chiral symmetry, time-reversal symmetry and particle-hole symmetry, respectively. The given symmetries lock a subset of the degeneracies to symmetry points in the time-momentum space which gives each system special topological properties. We evaluate the corresponding invariants with our approach and compare them to the chiral edge states of the Floquet spectrum via the bulk-edge correspondence.

TT 76.14 Thu 15:00 P2-OG1

Phase-coherent transport in 3D topological insulators encapsulated in hexagonal boron nitride — •Shaham Jafarpisheh[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], Bernd Beschoten[1,2], and Christoph Stampfer[1,2,4] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Helmholtz Virtual Institute for Topological Insulators (VITI), RWTH Aachen, 52072 Aachen, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan — [4]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

The spin-polarized current on the surface of topological insulators is a unique property which makes them promising materials for spintronic applications. However exposure to air and contaminations during the device fabrication easily destroys the surface states. This can be avoided by protecting the two surfaces of the TI layer with hexagonal boron nitride (hBN) crystals. In this work we show transport measurements in fully encapsulated BSTS layers in hBN. We fabricate Hall bars of the sandwich structures with 1-dimensional side contacts to the TI-layer. By measuring weak antilocalization (WAL) at low fields we extract phase-coherence lengths which are close to the values imposed by electron-electron interactions but limited by spin-flip scattering at temperatures below 1K.

TT 76.15 Thu 15:00 P2-OG1

Surface transport on thin semi-metallic films: The role of thickness and magnetic impurities — •Philipp Kröger, Marianna Siemens, Herbert Pfnür, and Christoph Tegenkamp — Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover

Bismuth has attracted a lot of interest because of its unique electronic properties such as low carrier concentrations and high carrier mobilities. Thereby, epitaxial growth of high-quality thin films opens new pathways to tailor the electronic properties further, e.g. by quantum confinement and alloy formation, giving rise to topologically non-trivial states in this material class. In this study we concentrate on Bi films grown on Si(111). Thin Bi(111) films become semiconducting due to the quantum-size-effect. Thus the peculiar spin texture of the surface states, induced by the Rashba effect, were studied directly by temperature and magnetic field dependent transport. Only at low temperatures (T<50 K) the conductance G turned out to be governed by surface states while at higher temperatures activated transport from bulk channels sets it. We have carefully analyzed the G(T)-behavior as a funnction of film thickness. With decreasing film thickness, the bulk gap increases, as expected due to the quantum size effect. However for thinner films the gap decreases. The reason is an interface-interface interaction which renormalizes strongly the Fermi surface.

TT 76.16 Thu 15:00 P2-OG1

Synthesis and characterization of the weak 3D topological insulator $Bi_{14}Rh_3I_9$ — •Ali Scherzad, Sebastian Witt, and Cornelius Krellner — Physikalisches Institut, Goethe University Frankfurt, 60438 Frankfurt am Main, Germany

The discovery of topological insulators generated high interests in the last decade. One of the main properties of topological insulators are surface currents and an isolated behavior inside the bulk. Motivated by recent Nobel Prize in physics for topological phases and based on previous work our goal was to synthesize novel types of topological insulators.

Here, we report the crystal growth of $Bi_{14}Rh_3I_9$ [1] in different crucible setups. Besides a larger muffle furnace, we used a vertical Bridgman furnace to obtain larger single crystals. An optimization of the crucible setup and temperature profile was necessary due to reactions of iodine with the crucible. All experiments were done under argon atmosphere and we tested Al_2O_3, quartz, Nb, graphite, and BN as crucible materials. The prepared crystals were characterized by using Laue-type diffraction, x-ray powder diffraction, EDX analysis and preliminary physical measurements down to 1.8 K.

[1] B. Rasche et al., Chem. Mater., 25, 2359-2364, (2013).

TT 76.17 Thu 15:00 P2-OG1

3D topological Kondo insulators: Slave-boson mean-field theory and fluctuations — •Soroush Arabi and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

Topological Kondo insulators (TKI) have recently been proposed as a new system where a gap at the Fermi energy and, subsequently, a non-trivial topological phase are created by strong correlations [1]. The present work investigates the influence of the finite life-time of the heavy Kondo quasiparticles on the stability of a TKI phase. Because of the strong spin-orbit (SO) coupling within the rare-earth 4f-orbitals of a heavy-fermion system, the local ground-state Kramers doublet involves mixing of spin and orbital degrees of freedom. This leads to a topological term in the hybridization of the 4f- and the conduction band [1]. Using slave-boson mean field theory [2], we calculate the band structure of a 3D bulk TKI. We then calculate the

layer-dependent band structure near a 2D surface of a 3D TKI. Finite quasiparticle life-time effects are incorporated by taking bosonic fluctuations about the mean field solution into account and by calculating the corresponding selfenergies. We aim at calculating characteristic, observable quantities, like the surface conductivity, including life-time effects.

[1] M. Dzero, et al., Ann. Rev. Cond. Matt. **7**, 249-280 (2016)
[2] V. Alexandrov, et al., Phys. Rev. Lett. **114**, 177202 (2015)

TT 76.18 Thu 15:00 P2-OG1

Scattering properties of electrons on TaAs Weyl Semimetal surfaces — •Steven Rendon Restrepo, Philipp Rüssmann, Phivos Mavropoulos, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

In the field of topological materials, the recent discovery of the Type-I Weyl semi-metals TaAs, NbP, NbAs and TaP came as a breakthrough. (B.Q.Lv et al. Nat. Phys. **11**, 724 (2015); S. Souma et al.,Phys. Rev. B **93**, 161112(R) (2015); Su-Yang Xu et al. Nat Phys,**11**, 748 (2015); Xu et al. Sci. Adv. 2015;1:e1501092).

In this class of materials, the valence and conduction band in the bulk touch at generic points in the Brillouin zone (Weyl nodes) due to a nontrivial Berry curvature. The Weyl nodes, always appearing in pairs, show a linear band dispersion in all three $\vec{k}$-directions. Their topological nature ultimately leads to topological surface states that take the form of open Fermi arcs.

In this presentation, I will discuss the band structure, spin-polarization and Fermi surfaces of the non-centrosymmetric TaAs family and present the relation of these properties to the scattering properties of electrons off surface defects. The calculations were performed using the density-functional-based, full-potential relativistic Korringa-Kohn-Rostoker Green-function method for electronic structure and impurity embedding.

Computational support from the JARA-HPC Centre at the RWTH Aachen University is acknowledged.

TT 76.19 Thu 15:00 P2-OG1

Planar Hall effect and anisotropic magnetoresistance from the surface states of disordered 3D topological insulators — •Henry Legg and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Zülpicher Straße 77, D-50937, Köln, Deutschland

In the presence of time-reversal symmetry electrons on the surface of a topological insulator cannot backscatter from disorder. A magnetic field parallel to the surface lifts this protection mechanism, enabling backscattering which is predominantly in the direction parallel to the magnetic field but retaining the Dirac physics of the surface. As a result the anisotropy of magnetoresistance parallel and perpendicular to **B** is a sensitive probe of the loss of topological protection when time-reversal symmetry is broken.

Using a self-consistent T-matrix approximation, including vertex corrections, we demonstrate how an in-plane magnetic field can dramatically alter the resistivity of a topological insulator's surface. We compare our theoretical results to experiments where the dependence on gate voltage provides an especially clear experimental signature of the scattering mechanism.

TT 76.20 Thu 15:00 P2-OG1

Gigantic negative magnetoresistance in the topological insulator $TlBi_xSb_{1-x}Te_2$ — •Oliver Breunig[1], Zhiwei Wang[1], Jonathan Lux[2], Achim Rosch[2], Alexey Taskin[1], and Yoichi Ando[1] — [1]Physics Institute II, University of Cologne — [2]Institute for Theoretical Physics, University of Cologne

Recently the phenomenon of negative magnetoresistance (MR) gains increasing interest in the context of the chiral anomaly in Weyl semimetals. Here, we present a new mechanism leading to a large negative MR that is related to disorder in a compensated topological insulator. We have grown single crystals of the topological insulator material $TlBi_xSb_{1-x}Te_2$ by a modified Bridgman technique. For intermediate values x we find a bulk-insulating state and a surprisingly strong negative MR reaching 98% at low temperature and in applied magnetic fields of 14 T. Based on transport data and numerical simulations we show that the increased conductivity at high fields is due to the magnetic field-enhanced percolation of localized electronic states.

TT 76.21 Thu 15:00 P2-OG1

Dynamics of Moving Majorana States and Disorder — •Qingyufei Terenz Feng, Zala Lenarcic, and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln 50937 Köln, Germany

A possible realization of quantum computers could base on the time dependent manipulation of qubits represented by Majorana states. Information stored in Majoranas is safe under manipulation in perfectly clean systems. However, this is not the case in realistic systems. We present a study of the dynamics of Majorana states operated by external gate potential in the presence of a single or multiple disorder. Our goal is to determine the limit on the velocity, at which operation can be performed. Starting from a non-interacting setup we aim to address the manipulation in interacting many-body localized systems as well.

TT 76.22 Thu 15:00 P2-OG1

Stretched exponential decay of Majorana edge modes in many-body localized Kitaev chains — •Florian Katsch[1], Leon Droenner[1], Markus Heyl[2], and Alexander Carmele[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Dynamics in correlated quantum matter, Nöthnitzer Str. 38, 01187 Dresden, Germany

We study a generic example of a system that fails to thermalize, namely a Kitaev chain with a bulk and topological edge-edge states [1, 2]. Therefore, the resilience of such Majorana modes in the presence of symmetry-breaking dissipation is investigated. Hence, both the loss and gain is described within a master equation framework, implying that the parity symmetry is violated. Considering a homogeneous system, it can be shown that the edge-edge correlation decays exponentially fast [3]. By including strong disorder to the system, the decay flattens and the Majorana mode survives longer. The result thus represents a first step to stabilize edge-edge states taking account of symmetry-breaking environments via a strong disorder mechanism closely connected to many-body localization.

[1] Pal *et al.*, Phys. Rev. B **82**, 174411 (2010)
[2] Kitaev, Phys. Usp. **44**, 131 (2001)
[3] Carmele *et al.*, Phys. Rev. B **92**, 195107 (2015)

TT 76.23 Thu 15:00 P2-OG1

Topological Quantum Wires with Balanced Gain and Loss — •Henri Menke and Moritz Hirschmann — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany

We study a one-dimensional topological superconductor, the Kitaev chain, under the influence of a non-Hermitian but $\mathcal{PT}$-symmetric potential. This potential introduces gain and loss in the system in equal parts. We show that the stability of the topological phase is influenced by the gain/loss strength and explicitly derive the bulk topological invariant in a bipartite lattice and compute the corresponding phase diagram using analytical and numerical methods. Furthermore we find that the edge state is exponentially localized near the ends of the wire despite the presence of gain and loss of probability amplitude in that region.

TT 76.24 Thu 15:00 P2-OG1

Transport Properties of Superconducting $In_xSn_{1-x}Te$ nano-plates and nano-ribbons — •Fan Yang, Zhiwei Wang, and Yoichi Ando — Institute of Physics II, University of Cologne, Zülpicher Straße 77, 50937 Cologne, Germany

$In_xSn_{1-x}Te$ nano-plates and nano-ribbons were grown on Si wafers coated with 300 nm SiO_2 via vapor-transport method. After the growth, the nano-plates and nano-ribbons were fabricated into devices. A sharp superconducting transition was observed at low temperatures. We also tried to fabricate tunneling junctions on the nano-plates and nano-ribbons, and the preliminary results are presented.

TT 76.25 Thu 15:00 P2-OG1

Low-temperature heat transport of the topological superconductor $Cu_xBi_2Se_3$ — •Lionel Andersen, Zhiwei Wang, Thomas Lorenz, and Yoichi Ando — II. Physikalisches Institut - Universität zu Köln, Germany

The topological insulator Bi_2Se_3 becomes superconducting when intercalated with copper. Recently the interest in this material was heightened by the confirmation of the topological superconductivity through observations of a rotational symmetry braking [1,2].

A manifestation of Majorana fermions is predicted to be a ballistic

surface heat transport [3]. This could provide a possibility of a direct macroscopic observation of these exotic surface states by standard heat transport measurements. For these measurements, a disentanglement of the contributions from phonons, surface Majorana fermions and bulk quasiparticles is required. In this poster, measurements of the heat transport of $Cu_xBi_2Se_3$ performed in a dilution refrigerator will be presented.

[1] K. Matano et al., Nat. Phys. **12**, 852 (2016)
[2] S. Yonezawa et al., Nat. Phys. DOI: 10.1038/NPHYS3907 (2016)
[3] L. Kouvenhoven and C. Beenakker, Nat. Phys. **12**, 618 (2016)

TT 76.26 Thu 15:00 P2-OG1

Zero-Temperature Bell Test in a Driven Mesoscopic Contact — •hongxin zhan[1], mihajlo vanevic[2], and wolfgang belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Department of Physics, University of Belgrade, 11158 Belgrade, Serbia

The standard Clauser-Horne-Shimony-Holt (CHSH) inequality [1] is known to fail in mesoscopic junctions at finite temperature [2]. Since this is due to the bidirectional particle flow, a similar failure is expected for an ac-driven junction. We develop a generalized Bell test which is suitable for ac driven system. Similar to the standard CHSH inequality, our Bell inequality cannot be violated when the detection time or the conductance are sufficiently large. Differently, our inequality cannot be violated for ac-driven system when the probability [3] of creating one or more electron-hole pairs is large. To determine the optimal ac bias for Bell test, we develop a quantitative criterion - similar to the Fano factor - for the probability of the creation of electron-hole pairs.

[1] N. M. Chtchelkatchev, G. Blatter, G. B. Lesovik, T. Martin, Phys. Rev. B **66**, 161320(2002).
[2] W. R. Hannes, M. Titov, Phys. Rev. B **77**, 115323(2008).
[3] M. Vanevic, Y. V. Nazarov, W. Belzig, Phys. Rev. Lett **99**, 076601(2007); Phys. Rev. B **78**, 245308(2008).

TT 76.27 Thu 15:00 P2-OG1

Full counting statistics analyzed by generalized factorial cumulants — •Philipp Stegmann, Stephan Weiss, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

We discuss the advantages of generalized factorial cumulants $C_{s,m}$ [1] yielding informations that are not accessible via ordinary cumulants commonly used in literature. Generalized factorial cumulants indicate the presence of correlations between transferred electrons [1,2]. Especially for short measuring-time intervals, higher-order tunneling events can be identified [2]. Moreover, generalized factorial cumulants can be utilized to obtain a lower bound of the system dimension and the full spectrum of relaxation rates. The generalized factorial cumulants give access to additional dimensions and relaxation rates hidden for ordinary cumulants [3]. Furthermore, coherent oscillations can be detected, although the oscillations do not influence commonly studied quantities as the charge current, zero- and finite-frequency noise, ordinary cumulants, and waiting times. We illustrate our findings for several Coulomb-blockade systems.

[1] P. Stegmann, B. Sothmann, A. Hucht, and J. König, PRB **92**, 155413 (2015).
[2] P. Stegmann and J. König, PRB **94**, 125433 (2016).
[3] P. Stegmann and J. König, arXiv:1611.02043.

TT 77: Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VI (joint session DS, HL, MA, MM, O, TT, organized by O)

Time: Thursday 16:00–18:30 Location: GER 38

Invited Talk TT 77.1 Thu 16:00 GER 38

Spectacular success of DFT in predicting novel topological phases — •Arun Bansil — Northeastern Univ, Boston USA

The revolutionary discovery of topological insulators has turned out to be the proverbial tip of the much larger iceberg of exotic phases of quantum matter driven by spin-orbit coupling effects. The consideration of electronic states protected by time-reversal, crystalline and particle-hole symmetries has led to the prediction of many novel materials that can support Weyl, Dirac and Majorana fermions, and to new types of topological crystalline and Kondo insulators, and quantum spin Hall insulators with large band gaps. The first-principles DFT-based band theory paradigm has been a key player not only in this discovery process but also in identifying salient characteristics of topological states, enabling direct and sharpened confrontation between theory and experiment. [1] I will discuss our recent theoretical work aimed at predicting topological materials and identify cases where the materials have been realized successfully. [2-10] I will also comment on the potential of topological materials as next generation platforms for manipulating spin and charge transport and other applications.

[1] Bansil, Lin and Das, Rev. Mod. Phys. 88, 021004 (2016). [2] Chang et al, Sci. Adv. 2, e1600295 (2016). [3] Huang et al., PNAS 113, 1180 (2016). [4] Zheng et al., ACS Nano 10, 1378 (2016). [5] Xu et al., Science 349, 613 (2015). [6] Zeljkovic et al., Nat. Mat. 14, 318 (2015). [7] He et al., Nat. Mat. 14, 577 (2015). [8] Xu et al., Nat. Phys. 11, 748 (2015). [9] Crisostomo et al., Nano Lett. 15, 6568 (2015). [10] Xu et al., Sci. Adv. 1, e1501092 (2015).

TT 77.2 Thu 16:30 GER 38

Interlayer excitons and Band Alignment in MoS_2/hBN/WSe_2 van der Waals Heterostructures — •Simone Latini — Technical University of Denmark, Copenhagen, Denmark

Van der Waals Heterostructures (vdWHs) are a unique platform for the realization of novel (opto)-electronic devices with embedded multifunctionality. Combining two-dimensional (2D) semiconductors with misaligned band edges can lead to the formation of photo-excited electrons and holes localized in distinct layers, which result into interlayer excitons. Understanding the energetics behind the formation of interlayer excitons is the first step towards the engineering of charge separation processes in photovoltaic devices and photodetectors. The contribution of our work is then twofold. (I) We calculate, for the first time, the interlayer exciton binding energies in complex vdWHs, specifically MoS_2/hBN/WSe_2 heterostructures, using a first-principles approach. The binding energy is of extreme technological importance as it is a measure of how strongly the electron-hole pair is bound and hence how easily it can be separated. (II) We obtain accurate electronic band edges at the interface between the layers of the vdWHs, a task which could not yet be accomplished with any available state of the art technique. Importantly, the accuracy of our calculated exciton binding energies and band edges is confirmed by a striking agreement with experimental data on photoluminesce of interlayer excitons in MoS_2/hBN/WSe_2 heterostructures.

TT 77.3 Thu 16:45 GER 38

Trionic effects in graphene nanoribbons and further nanomaterials — •Thorsten Deilmann and Kristian Sommer Thygesen — Center for Atomic-Scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Among low-dimensional materials armchair-edged graphene nanoribbons are very promising candidates with optical properties which are dominates by excitons. In the presence of additional charges, trions (i.e. charged excitons) can occur in the optical spectrum. With our recently developed first-principle many-body approach [1], we predict strongly bound trions in nanoribbons with decreasing binding energies of 660 to 140 meV for widths of 3.6 to 14.6 Å. We determine their optical spectra and identify several trions by their real-space wave functions.

[1] Phys. Rev. Lett. **116**, 196084.

TT 77.4 Thu 17:00 GER 38

Interface Structure Prediction using the Ab Initio Random Structure Searching Method — •Georg Schusteritsch and Chris Pickard — Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, U.K.

First-principles structure prediction of bulk materials is now routinely performed, however the field of predicting the atomic structure of in-

terfaces is still in its infancy. A detailed understanding of and ability to predict the atomic structure of interfaces is however of crucial importance for many technologies. Interfaces are very hard to predict due to the complicated geometries, crystal orientations and possible non-stoichiometric conditions involved and provide a major challenge to structure prediction. We present here the ab initio random structure searching (AIRSS) method and how it can be used to predict the structure of interfaces. Our method relies on generating random structures in the vicinity of the interface and relaxing them within the framework of density functional theory. The method is simple, requiring only a small set of parameters, and can be efficiently run on modern parallel computer architectures. We focus here on the prediction of grain boundaries, but application to heterostructure interfaces is straightforward. Examples for several grain boundary defects in technologically important materials will be presented: In particular grain boundaries in graphene, the prototypical two-dimensional material will be discussed, alongside with examples of grain boundaries in transition metal oxides, such as SrTiO3 and TiO2.

TT 77.5 Thu 17:15 GER 38

Predicting new materials and their properties with supercomputers: the example of perovskites — •Silvana Botti[1] and Miguel A.L. Marques[2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Can new materials with optimized properties be designed using supercomputers?

I will try to convince you through the example of the search of new perovskites that first-principles calculations can efficiently speed up the discovery of new materials.

Theoretical approaches based and going beyond density functional theory ally today accuracy and efficiency, and are therefore suitable tools for understanding the physics not only of simple perfect crystals, but also of nanostructured materials, doped semiconductors, interfaces, alloys, etc. As a result, ab initio simulations of spectroscopic properties can finally account for the complexity of "real" experimental samples, allowing accurate comparison of calculated and measured structural and excitation properties. The powerful combination of theoretical spectroscopy with high-throughput calculations, structural prediction and machine learning can therefore provide a precious guide to experimentalists in the search of new materials.

TT 77.6 Thu 17:30 GER 38

Spectral property prediction with artificial neural networks — •Annika Stuke[1], Milica Todorovic[1], Kunal Ghosh[2], Aki Vehtari[2], and Patrick Rinke[1] — [1]Department of Applied Physics, Aalto University, Finland — [2]Helsinki Institute of Information Technology, Department of Computer Science, Aalto University, Finland

The ability to efficiently design new and advanced optoelectronic materials is hampered by the lack of suitable methods to rapidly and accurately identify yet-to-be-synthesized materials that meet a desired application. To overcome such design challenges, a machine learning model based on a deep multi-task artificial neural network (ANN) is presented that can predict spectral properties of small organic molecules. The ANN is trained and validated on data generated by accurate state-of-the art quantum chemistry computations for diverse subsets of the GDB-13 and GDB-17 datasets [1,2]. The molecules are represented by a simple, easily attainable numerical description based on nuclear charges and cartesian coordinates and are mapped onto multiple excited-state properties simultaneously using a deep ANN trained by gradient descent and error backpropagation [3]. This on-demand prediction model can be used to infer spectral properties of various candidate molecules in an early screening stage for new optoelectronic materials at negligible computational cost, thereby completely bypassing conventional laborious approaches towards materials discovery.

[1] L. C. Blum et al., J. Am. Chem. Soc. 2009, 131, 8732, [2] R. Ramakrishnan et al., Scientific Data 2014, 1, 140022, [3] G. Montavon et al., New J. Phys. 2013, 15, 095003

TT 77.7 Thu 17:45 GER 38

Machine-Learning Based Interatomic Potential for Amorphous Carbon — •Volker Deringer and Gábor Csányi — University of Cambridge, Cambridge, UK

Machine-learning based interatomic potentials are currently of growing interest in the solid-state theory communities, as they enable materials simulations with close-to DFT accuracy but at much lower computational cost. Here, we present such an interatomic Gaussian approximation potential (GAP) model for liquid and amorphous carbon. We first discuss the maximum accuracy that any finite-range potential can achieve in carbon structures; then, we show how a hierarchical set of two-, three-, and many-body structural descriptors can be used to fit a GAP that indeed reaches the target accuracy. The new potential yields accurate energetic and structural properties over a wide range of densities; it also correctly captures the structure of the liquid phases, at variance with state-of-the-art empirical potentials. Exemplary applications to surfaces of "diamond-like" tetrahedral amorphous carbon (ta-C) will be presented, including simulations of high-temperature surface reconstructions ("graphitization"). The method appears to be promising for realistic and accurate simulations of nanoscale amorphous carbon structures.

TT 77.8 Thu 18:00 GER 38

High-throughput computational search for new high mobility transparent (semi)conducting materials — •Geoffroy Hautier[1], Joel Varley[2], Anna Miglio[1], David Waroquiers[1], Viet-Anh Ha[1], and Gian-Marco Rignanese[1] — [1]Université catholique de Louvain, Louvain-la-Neuve, Belgium — [2]Lawrence Livermore National Laboratory

Transparent conducting oxides (TCMs) are large band gap materials (to favor transparency) doped with electrons (n-type) or holes (p-type). TCMs are essential to many technologies from solar cell to transparent electronics and there is currently a large effort towards the discovery of new TCMs. I will present the results of a high-throughput computational search for new TCMs especially directed at p-type materials. Focusing on low effective masses (leading to high mobility), large band gaps and dopability, I will show how thousands of compounds can be screened using various ab initio techniques (from density functional theory to GW) to find new potential high performance TCMs. I will discuss several unsuspected compounds with promising electronic structures and when available link our findings to experimental results. Beyond the description of those novel TCM candidates, I will chemically rationalize our findings, highlighting several design strategies towards the development of future high mobility TCMs.

TT 77.9 Thu 18:15 GER 38

Cross-validation in the cluster expansion method — •Axel Hübner, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

The cluster expansion technique allows the construction of model Hamiltonians for an efficient evaluation of the total energy of alloys. This technique relies on a fit to a small set of *ab-initio* calculations for selected atomic configurations. Key aspects to maximize the predictive performance of the model are the selection of a set of basis functions, i.e. clusters, and of configurations. To achieve this, the cross-validation technique is typically used [1]. In this work, an analytical formula for the calculation of the leave-many-out cross-validation score (CV) is derived. This formula exhibits numerical instabilities, whose analytical properties yield a criterion for structure selection in cluster expansions. Moreover, a relation between the noise in the data and the CV is outlined. This leads to a tool which allows us to estimate, for a given noise level, the size of the ab-initio data set upon which no improvements of the model are obtained. These results are exemplified for a cluster expansion of the thermoelectric clathrate alloy $Ba_8Al_xSi_{46-x}$, calculated with the `CELL` package [2].

[1] A. van d. Walle *et al.*, Journal of Phase Equilibria 23 (2002), Aug., Nr. 4

[2] M. Troppenz *et al.*, submitted (2016); S. Rigamonti *et al.*, in preparation.

TT 78: Quantum Optics at the Nanoscale: From Fundamental Physics to Quantum Technologies (joint session HL, DS, O, and TT, organized by DS)

Time: Thursday 17:00–17:30 Location: CHE 91

TT 78.1 Thu 17:00 CHE 91

Sensing weak radio-frequency radiation by pulsed Autler-Townes spectroscopy — Timo Joas, Andreas M. Waeber, Georg Braunbeck, and •Friedemann Reinhard — TU München, Walter Schottky Institut and Physik-Department

Nano-emitters have shaped a new era of quantum optics, serving as convenient single photon sources, e.g. to launch surface plasmons [1,2] or to build long-distance entanglement [3]. So far, they have mostly been used in the optical (100THz) domain.

Here we employ a nano-emitter and a quantum-optical protocol to detect weak radiation in the radio-frequency (GHz) range. Our scheme is based on Autler-Townes spectroscopy [4]. We extend this technique to a pulsed protocol, which greatly improves spectral resolution, sensitivity and robustness to experimental fluctuations.

We demonstrate our approach on a NV center in diamond, where it might enable various applications. Specifically, we consider radio-astronomy, ultrasound detection and spin-phonon coupling.

[1] A.V. Akimov et al., Nature 450, 402 (2007)
[2] R. Kolesov et al., Nature Physics 5, 470 (2009)
[3] B. Hensen et al., Nature 526, 682 (2015)
[4] J.A. Gordon et al., Appl. Phys. Lett. 105, 024104 (2014)

TT 78.2 Thu 17:15 CHE 91

Free-electron quantum optics — •Katharina E. Priebe, Christopher Rathje, Armin Feist, Sergey V. Yalunin, Sascha Schäfer, and Claus Ropers — 4th Physical Institute - Solids and Nanostructures, University of Göttingen, Göttingen, Germany

Besides being a powerful tool for time-resolved measurements of nanoscale dynamics, ultrafast transmission electron microscopy (UTEM) serves as an ideal test bench for quantum optical experiments studying the interaction with free-electron beams. Specifically, inelastic scattering between the electrons and strong optical near-fields [1] allows for a coherent manipulation of the electron quantum state [2]. The optical near-field imprints a sinusoidal phase modulation on the electron wavefunction, which is manifest in a comb of sidebands in the electron kinetic energy distribution. In this contribution, we will demonstrate how multiple near-fields can be employed to coherently control the free-electron momentum superposition states [3,4]. Furthermore, dispersive propagation translates the phase modulation into a density modulation: the electron wavefunction is self-compressed into a train of attosecond bursts. This temporal structuring of free-electron beams may find applications in electron microscopy with attosecond resolution.

[1] B. Barwick *et al.*, Nature, **462**, 902 (2009).
[2] A. Feist *et al.*, Nature, **521**, 200-203 (2015).
[3] K. E. Echternkamp *et al.* Nat. Phys **12**, 1000-1004 (2016).
[4] K. E. Priebe *et al.* In preparation.

TT 79: Transport: Spintronics, Spincalorics and Magnetotransport (jointly with DS, HL, MA)

Time: Friday 9:30–11:30 Location: HSZ 03

TT 79.1 Fri 9:30 HSZ 03

Search for magneto-hydrodynamics in the delafossite metals $PdCoO_2$ and $PtCoO_2$ — •Nabhanila Nandi[1], Pallavi Kushwaha[1], Seunghyun Khim[1], Philip J.W. Moll[1], Burkhard Schmidt[1], Thomas Scaffidi[2], Markus König[1], and Andrew P. Mackenzie[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Department of Physics, University of California, Berkeley, California 94720, USA — [3]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom

Electrical resistance is conventionally determined by the momentum-relaxing scattering of electrons by the host solid and its excitations. Hydrodynamic fluid flow through channels, in contrast, is determined by geometrical factors, boundary scattering and the viscosity of the fluid, which is governed by momentum-conserving internal collisions. In almost all known materials, however, the signatures of viscosity in electron flow cannot be resolved, because the rate of momentum-relaxing collisions dominates that of the momentum-conserving ones that give the viscous term. In previously published work, we reported experimental evidence that there is a regime in restricted channels of the ultra-pure two-dimensional delafossite metal $PdCoO_2$ in which the resistance has a large viscous contribution. In this talk I will report on our current work in which we extend our experiments to magneto-hydrodynamics, discussing data both from $PdCoO_2$ and a second delafossite metal, $PtCoO_2$.

TT 79.2 Fri 9:45 HSZ 03

Fe_3O_4 thin films: controlling and manipulating an elusive quantum material — •xionghua liu, chun-fu chang, aurora diana rata, alexander christoph komarek, and liu hao tjeng — Max Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, 01187 Dresden, Germany

Fe_3O_4 (magnetite) is one of the most elusive quantum materials and at the same time one of the most studied transition metal oxide materials for thin film applications. The theoretically expected half-metallic behavior generates high expectations that it can be used in spintronic devices. Yet, despite the tremendous amount of work devoted to preparing thin films, the enigmatic first order metal-insulator transition and the hall mark of magnetite known as the Verwey transition, is in thin films extremely broad and occurs at substantially lower temperatures as compared to that in high quality bulk single crystals.

In this work, we investigate systematically the effect of oxygen stoichiometry, thickness, strain, and microstructure on the Verwey transition in epitaxial Fe_3O_4 thin films on a variety of substrates. We have been able to determine the factors that affect negatively the Verwey transition in thin films. We have succeeded in finding and making a particular class of substrates that allows the growth of magnetite thin films with the Verwey transition as sharp as in the bulk. Moreover, we are now able to tune the transition temperature and, using tensile strain, increase it to substantially higher values than in the bulk.

TT 79.3 Fri 10:00 HSZ 03

Spin-switching via quantum dot spin valves — •Niklas M. Gergs[1], Scott A. Bender[1], Rembert A. Duine[1,2], and Dirk Schuricht[1] — [1]Institute for Theoretical Physics, Utrecht University, Utrecht, The Netherlands — [2]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

We theoretically investigate a spin-valve transistor setup, ie, correlated transport through a quantum dot positioned between two spin-polarised nano magnets. This causes the dynamical generation of a magnetic field on the dot even in the absence of external fields [1].

Here we consider the back action of the quantum dot onto the attached nano magnets via exerted spin torques. This may be used to switch the nano magnets reliably from a parallel to an anti-parallel alignment and vice versa. All operations are done in the Coulomb-blockade regime of the quantum dot, so that the charge transport through the setup is strongly suppressed.

[1] M. Braun, J. König, J. Martinek, Phys. Rev. B 70, 195345 (2004)

TT 79.4 Fri 10:15 HSZ 03

Strong non-equilibrium effects in spin torque systems — •Tim Ludwig[1], Igor S. Burmistrov[2,3], Yuval Gefen[4], and Alexander Shnirman[1] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]L.D. Landau Institute for Theoretical Physics RAS, Kosygina street 2, 119334 Moscow, Russia — [3]Laboratory for Condensed Matter Physics, National Research University Higher School of Economics, 101000 Moscow, Russia — [4]Department of Condensed Matter Physics, Weizmann Institute of Science, 76100 Rehovot, Israel

We consider a problem of persistent magnetization precession in a single domain ferromagnetic nano particle under the driving by the spin-transfer torque [1]. We find that the adjustment of the electronic distribution function in the particle renders this state unstable. Instead, abrupt switching of the spin orientation is predicted upon increase of the spin-transfer torque current. On the technical level, we derive an effective action of the type of Ambegaokar-Eckern-Schön action for the coupled dynamics of magnetization (gauge group SU(2)) and voltage (gauge group U(1)).
[1] T. Ludwig, I. S. Burmistrov, Y. Gefen, and A. Shnirman, arXiv:1610.09944 (2016)

TT 79.5 Fri 10:30 HSZ 03

Spin-charge coupled dynamics driven by a time-dependent magnetization — •Sebastian Tölle[1], Ulrich Eckern[1], and Cosimo Gorini[2] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Faculty of Physics, University of Regensburg, 93040 Regensburg, Germany

The spin-charge coupled dynamics in a thin, magnetized metallic system are investigated. The effective driving force acting on the charge carriers is generated by a dynamical magnetic texture, which can be induced, e.g., by a magnetic material in contact with a normal-metal system. We consider a general inversion-asymmetric substrate/normal-metal/magnet structure, which, by specifying the precise nature of each layer, can mimick various experimentally employed setups. Inversion symmetry breaking gives rise to an effective Rashba spin-orbit interaction. We derive general spin-charge kinetic equations which show that such spin-orbit interaction, together with anisotropic Elliott-Yafet spin relaxation, yields significant corrections to the magnetization-induced dynamics. To highlight their physical meaning, the spin pumping configuration of typical experimental setups is analyzed in detail. In the two-dimensional limit the build-up of a DC voltage is dominated by the spin galvanic (inverse Edelstein) effect. A measuring scheme that could isolate this contribution is discussed.

TT 79.6 Fri 10:45 HSZ 03

Emergent magnetic ordering in transition metal atomic contacts — •Martin Keller, Florian Strigl, Elke Scheer und Torsten Pietsch — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

MD simulations and DFT calculations predict the development of local magnetic order at reduced dimensions in some paramagnetic transition metals (Pt, Pd, Ir), especially in atomic configurations [1,2,3]. This unusual property allows us to investigate the influence of the local magnetic properties on the conductance of atomic contacts without the effect of magnetic leads. Therefore atomic contacts of these metals are a model system to understand the origin of magnetoconductance and the role of spin-polarization of the conduction electrons. Herein we discuss recent results of Pt, Pd and Ir in the context of a microscopic model that successfully describes the observed magnetoconductance signature in these atomic contacts and chains [4]. Additionally, electronic transport spectroscopy is used to evaluate magnetic excitations in the electronic system of the contact, i.e. the presence of i) a zero-bias anomaly which is described by Kondo physics and ii) conductance fluctuations in the atomic contact, which indicate the formation of a magnetically ordered state. We will compare the three transition metals with respect to their different electronic structure and the role of spin-orbit coupling in the contacts.
[1] Phys. Rev. Lett. 92, 057201 (2004)
[2] Phys. Rev. B 78, 014423 (2008)
[3] Phys. Rev. B 81, 054433 (2010)
[4] Nature Comm. 6, 6172 (2015); Phys. Rev. B 94, 144431 (2016)

TT 79.7 Fri 11:00 HSZ 03

Electron transport through the helical systems: chiral magnetoresistance effect — •Volodymyr V. Maslyuk, Rafael Gutiérrez, and Gianaurelio Cuniberti — Institute for Material Science and Max Bergmann Center for Biomaterials, Dresden University of Technology, Hallwachstr. 3, 01069 Dresden, Germany

Recently, the chirality-induced spin selectivity (CISS) effect [1] has been discovered in which electron transport through systems with helical symmetry shows the different transmission for the electrons with different spin-polarizations. In this work, we show that CISS can be utilized in the new class of magnetic field sensors via novel chiral magnetoresistance effect (CMR) [2]. We present a theoretical investigation of the electron transport through the poly-GLY in helical form placed between one magnetic and one nonmagnetic leads by using the DFT and NEGF approach. We obtain that MR of the order 2
[1] Göhler B., Hamelbeck V., Markus T. Z., Kettner M., Hanne G. F., Vager Z., Naaman R., and Zacharias H., Science 331, 894 (2011)
[2] Kiran V., Mathew S.P., Cohen S.R., Delgado I.H., Lacour J., Naaman R., Adv. Mater. 28, 1957 (2016)

TT 79.8 Fri 11:15 HSZ 03

A Landauer-Büttiker approach for hyperfine mediated electronic transport in the integer quantum Hall regime — •Aniket Singha[1], M. Hamzah Fauzi[2], Yoshiro Hirayama[2], and Bhaskaran Muralidharan[1] — [1]Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India — [2]Graduate School of Science, Tohoku University, Aoba-ku, Sendai-980-8578, Japan

The interplay of spin-polarized electronic edge states with the dynamics of host nuclei in quantum Hall systems presents rich and non-trivial transport physics. Here, we develop a Landauer-Büttiker approach to understand various experimental features observed in integer quantum Hall set ups featuring quantum point contacts. Such approach entails a phenomenological description of spin resolved inter-edge scattering induced via hyperfine assisted electron-nuclear spin flip-flop processes along with a self consistent simulation framework between the nuclear spin dynamics and edge state electronic transport in order to gain insights into the nuclear polarization effects on electronic transport vice-versa. In particular, we show that the hysteresis noted experimentally in the conductance-voltage trace as well as in the resistively detected NMR lineshape results from a lack of quasi-equilibrium between electronic transport and nuclear polarization evolution. In addition, we present circuit models to further facilitate a clear understanding of the electronic transport processes occurring near the quantum point contact.

TT 80: Low-Dimensional Systems: Oxide Hetero-Interfaces

Time: Friday 9:30–11:00 Location: HSZ 103

TT 80.1 Fri 9:30 HSZ 103

Metal-Insulator Transition in $CaVO_3$ Thin Films from DFT+DMFT — •Sophie Beck, Gabriele Sclauzero, and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

The wide variety of interesting phenomena and functionalities of complex oxide thin films and heterostructures is generally determined by a number of different factors, such as substrate-induced epitaxial strain, dimensional confinement, interface-related effects, or defects. Here, we investigate the effects of epitaxial strain, dimensional confinement, as well as interface and surface effects on the electronic properties of the correlated metal $CaVO_3$ using a combination of density functional theory (DFT) and dynamical mean-field theory (DMFT). We show that tensile epitaxial strain can induce a metal-insulator transition in $CaVO_3$, and we demonstrate that this strain effect cooperates with a similar tendency originating from the finite thickness of the thin film. The latter effect, however, is quantitatively only relevant in the ultra-thin limit. Furthermore, we also address the influence of the substrate-film interface in $CaVO_3/LaAlO_3$ heterostructures.

TT 80.2 Fri 9:45 HSZ 103

Electronic and orbital reconstruction in $La_2CuO_4/LaNiO_3$ superlattices — •Benjamin Geisler[1], Friederike Wrobel[2], Eva Benckiser[2], Bernhard Keimer[2], and Rossitza Pentcheva[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg, Germany — [2]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

Artificial transition metal oxide heterostructures can display exotic characteristics notably different from their bulk components. In a combined experimental and theoretical study we report on superlattices formed by the parent compound of cuprate superconductors La_2CuO_4 (d^9) and the correlated metal $LaNiO_3$ (formal d^7). TEM reveals high

quality $(La_2CuO_4)_N/(LaNiO_3)_M(001)$ structures ($N = 2, 3$; $M = 4$). Density functional calculations with on-site correlation show that the electrostatic doping due to an extra LaO layer at the interface is exclusively accommodated in the $LaNiO_3$ region, while the electronic and magnetic properties of the La_2CuO_4 part remain bulk-like. This is consistent with our Ni L-edge XAS measurements which provide evidence for Ni^{2+} in addition to the expected Ni^{3+}. In addition, a charge disproportionation arises at the Ni sites that drives a metal-to-insulator transition in the interface layers and is reflected also by the magnetic moments and the octahedral volumes. The simulations show a preference for a layerwise AFM order of the Ni moments but with a net total moment, which agrees with our XMCD measurements. A Ni orbital polarization of $\sim 6\%$ in favor of $3d_{z^2}$ arises near the interfaces.

Funding by the DFG within TRR 80 (G1, G3, G8) is acknowledged.

TT 80.3 Fri 10:00 HSZ 103

Anisotropic electrical transport at the Al_2O_3-$SrTiO_3$ interface — •Karsten Wolff[1], Roland Schäfer[1], Hilbert von Löhneysen[1,2], Matthieu le Tacon[1], and Dirk Fuchs[1] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe

At the interface of TiO_2-terminated $SrTiO_3$ and amorphous Al_2O_3, we observe anisotropic electrical transport behavior of the two dimensional electron system (2DES). Temperature and magnetic field dependence of the sheet resistance R_s is measured for various current directions with respect to the [100] direction of $SrTiO_3$. Below 30 K, R_s shows a distinct anisotropic behavior which can be attributed to anisotropic defect scattering. In addition, application of magnetic field parallel to the 2DES results in a non-crystalline anisotropy which we will discuss in terms of spin-orbit coupling.

TT 80.4 Fri 10:15 HSZ 103

2DEGs in binary oxides studied by ARPES: *s* vs. *d* orbitals and electron-phonon coupling — •Tobias C. Rödel[1,2,3], Franck Fortuna[1], François Bertran[2], Patrick Le Fèvre[2], and Andrés Felipe Santander-Syro[1] — [1]CSNSM, Univ. Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, 91405 Orsay, France — [2]Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin-BP48, 91192 Gif-sur-Yvette, France — [3]LPV, Physics and Material Science, University of Luxembourg, L-4422 Belvaux, Luxembourg

Two-dimensional electron gases (2DEGs) in $SrTiO_3$ attracted a lot of interest after the initially discovery at the $LaAlO_3/SrTiO_3$ interface due to its controversial origin and various different ground states (*e.g.* superconductivity, magnetism) which are tunable by a gate-voltage. We demonstrated that 2DEGs can be created in various other perovskite oxides using a simple Al-capping. This technique works also for non-perovskite systems and we studied the 2DEGs in the binary oxides TiO_2 and ZnO by angle-resolved photoelectron spectroscopy. One major difference between the two systems is that the orbital character of the 2DEG is either *s*-type (ZnO) or *d*-type (TiO_2) and the resulting differences in the measured electronic structure of the 2DEG will be discussed. Recently, electron-phonon coupling in the 2DEG in $SrTiO_3$ was the focus of various studies. Similar to $SrTiO_3$, the transition from a polaron gas to a Fermi liquid can be observed in the two binary oxides depending on the charge carrier density. We will focus on the characterization of electron-phonon coupling for high charge densities.

TT 80.5 Fri 10:30 HSZ 103

Tunable redox-created 2DES at the EuO/$SrTiO_3$ interface — •Patrick Lömker[1], Tobias Rödel[2], Timm Gerber[1], Patrick LeFevre[3], Francois Bertran[3], Emmanouil Frantzeskakis[2], Andrés Santander-Syro[2], and Martina Müller[1,4] — [1]Forschungszentrum Jülich GmbH, PGI-6, Jülich, Germany — [2]CSNSM, CNRS/IN2P3 and Université Paris-Sud, Orsay, France — [3]Synchrotron SOLEIL, Saint-Aubin, France — [4]Universität Duisburg-Essen, Duisburg, Germany

Two-dimensional electron systems (2DES) of transition metal oxides are of interest in the research for novel properties of oxidic systems. Well known systems, such as $LaAlO_3/SrTiO_3$, are challenging to fabricate in a consistent way for varying deposition techniques. A recent study enabled the fabrication of 2DES in a experimentally simple way by utilizing a non-magnetic reducing agent. [1]

In our study, we use Eu metal as the reducing agent in order to redox-create EuO. EuO belongs to the rare material class of magnetic insulators. This property combination makes EuO interesting for fundamental spintronics studies, e.g. decoupling spin from charge currents or electrical sensing of magnetic properties.

The EuO/$SrTiO_3$ interface is studied using *in-situ* ARPES. *Ex-situ* magnetometry is utilized to analyze the ferromagnetic properties of 1-2ML EuO films and element-selective XPS depth-profiling probes the thickness of the 2DES region. We find a 2DES in which electrical and ferromagnetic properties can be controlled simultaneously.

[1] Rödel, Advanced Materials 28, 1976-1980 (2016).

TT 80.6 Fri 10:45 HSZ 103

Band alignment and charge transfer in complex oxide interfaces — •Zhicheng Zhong and Philipp Hansmann — Max Planck Insitute Solid State Research , Stuttgart

Synthesis of transition metal heterostructures presents one of the most vivid fields in the design of novel functional materials. We propose a simple scheme to predict band alignment and charge transfer in complex oxide interfaces. For semiconductor heterostructures band alignment rules like the well known Anderson or Schottky-Mott rule are based on comparison of the work function of the bulk components. This scheme breaks down for oxides due to the invalidity of a single workfunction as it was recently shown. We propose a new scheme which is built on a continuity condition of valence states originating in the compounds' shared network of oxygen. It allows for the prediction of sign and relative amplitude of the intrinsic charge transfer, taking as input only information about the bulk properties of the components. We support our claims by numerical density functional theory simulations as well as (where available) experimental evidence. Specific applications include i) controlled doping of $SrTiO_3$ layers with the use of 4*d* and 5*d* transition metal oxides and ii) the control of magnetic ordering in manganites through tuned charge transfer.

TT 81: Correlated Electrons: Chiral Magnets

Time: Friday 9:30–10:30 Location: HSZ 304

TT 81.1 Fri 9:30 HSZ 304

Stability of Skyrmion in Chiral Magnets — •Alfonso Chacon[1], Marco Halder[1], Jonas Kindervater[2], Andreas Bauer[1], Sebastian Mühlbauer[3], and Christian Pfleiderer[1] — [1]Technische Universität München, München, Germany — [2]John Hopkins University, Baltimore, USA — [3]Heinz Maier-Leibnitz Zentrum, Garching, Germany

The non-trivial topological winding of skyrmions in chiral magnets distinguishes them from conventional forms of magnetic order and micromagnetic textures. This topological protection of skyrmions promises a new route to advanced non-volatile high density data storage devices. We report a detailed study of the stability and the decay of skyrmion lattices in chiral magnets when prepared in a metastable state. We consider possible decay mechanisms and discuss the underlying energy scales associated with the topological protection.

TT 81.2 Fri 9:45 HSZ 304

Nanostructured MnSi - physical and electronic characterization — •David Schroeter[1], Nico Steinki[1], Alexander Fernández Scarioni[2], Hans Werner Schumacher[2], Stefan Süllow[1], and Dirk Menzel[1] — [1]Technische Universität Braunschweig, Institut für Physik der Kondensierten Materie, D-38106 Braunschweig, Germany — [2]Physikalisch Technische Bundesanstalt, D-38116 Braunschweig, Germany

Manganese silicide (MnSi), which crystallizes in the non-centrosymmetric cubic B20 structure, shows intriguing magnetic properties involving the existence of skyrmions in the magnetic phase diagram. Since MnSi as bulk crystal has been intensively investigated using a multitude of different experimental techniques, the magnetic and transport properties are well understood. In contrast, measurements of the electronic transport in MnSi thin films reported

in literature show irregular and sample dependent results.

In this situation, we have set out to reinvestigate the (magneto)resistivity and Hall effect in MnSi thin films. We have carefully performed Hall and resistivity experiments on nanostructured MnSi thin films and have analyzed the electronic transport properties in Hall geometries of various size to determine the intrinsic behavior. We compare bulk, thin film and nanostructure data and discuss our results in consideration of the structural and morphologic characterization of the samples.

TT 81.3 Fri 10:00 HSZ 304

Mott physics of the frustrated triangular lattice Hubbard model with SU(3) fermions and fluxes — •Carolin Boos[1], Frédéric Mila[2], and Kai Schmidt[1] — [1]FAU Erlangen-Nürnberg, Deutschland — [2]EPF Lausanne, Schweiz

Ultra cold atoms allow to study fermions with SU(N)-symmetry on artificial lattices with fluxes. The theoretical description of such systems is given by the SU(N)-Hubbard model. In the strong-coupling limit the fermions exhibit a Mott phase, that can be described by effective spin models. Here we go beyond the leading-order Heisenberg model and use a linked-cluster expansion up to order five to derive effective models for the square and triangular lattice for general N and flux Φ.

In this work we investigate the Mott phase of the frustrated triangular lattice Hubbard model for N = 3 but general flux Φ by applying exact diagonalization on the effective spin model. To this end we exploit the full SU(3) symmetry allowing to treat periodic clusters up to 21 sites. Tuning the value of the flux Φ, we find a rich Mott phase including ordered and chiral phases.

TT 81.4 Fri 10:15 HSZ 304

Chiral Spin Liquids in Frustrated Quantum Magnetism — •Alexander Wietek — Universität Innsbruck

Topological states of matter are of of fundamental interest in contemporate condensed matter physics. The Fractional Quantum Hall effect is the main experimental system where this physics can be observed in a laboratory. The question remains whether also different systems might exhibit topological ordering. Candidate systems are certain frustrated quantum magnets. Chiral Spin Liquids are a lattice analogue of Fractional Quantum Hall Effect wave functions. These wavefunctions have been envisioned in 1987 but only very recently several simple local lattice models have been proposed realizing chiral spin liquid physics. In this talk I will introduce chiral spin liquids, discuss their relation to the Fractional Quantum Hall effect and present recent numerical studies that provide conclusive evidence for the emergence of this exotic state of matter in frustrated extended Heisenberg models.

[1] P. Nataf, M. Lajkó, A. Wietek, K. Penc, F. Mila, and A. M. Läuchli, Phys. Rev. Lett. 117 167202 (2016)
[2] A. Wietek, A. Sterdyniak, and A. M. Läuchli, Phys. Rev. B 92 125122 (2015)
[3] A. Wietek and A. M. Läuchli, arXiv:1604.07829 [cond-mat]

TT 82: Quantum Information Systems (joint session HL, MA, TT, organized by HL)

Time: Friday 9:30–11:15 Location: POT 81

TT 82.1 Fri 9:30 POT 81

Resonant driving of silicon vacancies in 4H-SiC — •Matthias Widmann[1], Roland Nagy[1], Matthias Niethammer[1], Ilja Gerhardt[1,2], Ivan G. Ivanov[3], Sophia Economou[4], Takeshi Oshima[5], Nguyen Tien-Son[3], Cristian Bonato[6], Sang-Yun Lee[7], Erik Janzén[3], and Jörg Wrachtrup[1,2] — [1]3rd Institute of Physics, IQST and Research Center SCOPE, Stuttgart — [2]Max-Planck Institute, Stuttgart — [3]Department of Physics, Chemistry and Biology, Linkoeping University — [4]Department of Physics, Virginia Tech, Blacksburg — [5]National Institutes for Quantum and Radiological Science and Technology (QST), Takasaki — [6]Institute of Photonics and Quantum Science, Heriot-Watt University — [7]Center for Quantum Information, Korea Institute of Science and Technology (KIST), Seoul

Spins associated to atomic scale defects in solids are attractive as sensitive probes and are promising candidates for quantum information processing (QIP) [1]. Our research is based on spin defects in silicon carbide (SiC), a technologically-relevant wide-bandgap semiconductor which offers spin-active defects with long coherence times at room temperature [2]. In this work, we extend our previous single spin study [2] by investigating optical and spin properties of the silicon vacancy in 4H-SiC via resonant optical and spin driving and discuss their potential use for quantum computing and quantum communication [3].

[1] F. Jelezko et al, PRL 100, (2012).
[2] M. Widmann et al, Nat. Mater 14 (2015).
[3] Ö. Soykal et al, PRB 93 (2016).

TT 82.2 Fri 9:45 POT 81

Cavity mediated entanglement generation between the electron spins of two NV$^-$ centers — •Vladislav Shkolnikov[1], 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 negatively charged 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. The excitation of the first NV, generated by the laser, can later be emited into the cavity and then reabsorbed by the second NV. The excited states in this process are only virtually occupied and it allows to generate entangling gate between the NV-centers, that is not limited by the excited state lifetime. We derive an analytical model for the case when spin-spin interaction in the excited state can be neglected and perform a numerical simulation taking it into account. We predict entangling gates with the operation time 500 ns, which is much smaller than spin coherence time in the NVs. In combination with previously demonstrated single-qubit gates, CPHASE allows for arbitrary quantum computations.

TT 82.3 Fri 10:00 POT 81

High-resolution NMR spectroscopy on small spin ensembles using a hybrid spin sensor — •Matthias Pfender[1], Nabeel Aslam[1], Philipp Neumann[1], Hitoshi Sumiya[4], Shinobu Onoda[5], Carlos A. Meriles[3], Junichi Isoya[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart — [2]Research Center for Knowledge Communities, University of Tsukuba — [3]Department of Physics, CUNYCity College of New York — [4]Sumitomo Electric Industries Ltd., Itami, Japan — [5]Takasaki Advanced Radiation Research Institute, Takasaki, Japan

In the last few years, the nitrogen-vacancy defect in diamond has emerged as an exceptional quantum sensor for magnetic and electric fields, capable of detecting proton spins outside the diamond. However, the performance of the NV electron spin alone limits the achievable resolution of an NV NMR spectroscopy experiment to about 200 Hz [2,3]. By using the NV's inherent nitrogen nuclear spin we form a robust hybrid quantum sensor, capable of performing NMR spectroscopy on nanometer sized samples. The hereby obtained spectra are not limited by the electron spin lifetimes, but rather by the sample spins. We perform NMR spectroscopy on spins inside and outside the diamond, reaching a frequency resolution of 10 Hz and 100 Hz, respectively, enough to extract structural information of the molecule.

[1] Staudacher, T. et al. Science 339, 561-563 (2013).
[2] Kong, X., Stark, A., Du, J., McGuinness, L. P. & Jelezko, F. Phys. Rev. Applied 4, 24004 (2015).
[3] Zaiser, S. et al. Nat Commun 7, 12279 (2016).

Coffee Break

TT 82.4 Fri 10:30 POT 81

Defect Engineering in Silicon Carbide — •Christian Kasper[1], Hannes Kraus[1,2], Dimitrij Simin[1], Yoshinori Suda[3], Takeshi Ohshima[2], Wataru Kada[3], Shunsuke Kawabata[3], Tomoya Honda[2,4], Yasuto Hijikata[4], Georgy Astakhov[1], and Vladimir Dyakonov[1,5] — [1]Exp. Physics VI, Julius Maximilian University of Würzburg — [2]National Institutes for Radiological Science and Technology(QST, formerly Japan Atomic Energy Agency), Takasaki, Japan

— [3]Gunma University, Kiryu, Japan — [4]Saitama University, Saitama, Japan — [5]ZAE Bayern, Würzburg

Because of their long spin lifetime[1] and their unique spin-preserving optical pumping mechanism[2], quantum centers in silicon carbide (SiC) are promising candidates for spin based quantum information processing. Well known methods to produce one of these quantum center species, the silicon vacancy, homogeneously in the bulk are electron or neutron[3] irradiation. In contrast, a method to implant silicon vacancies at a specific position would be a huge improvement in terms of defect engineering.

In this study, the generation of silicon vacancies in bulk SiC as a result of proton irradiation can be verified. By the use of confocal microscopy, we show that the implantation depth is tunable by varying the irradiation energy. Further, we verify that by proton beam writing silicon vacancies can be implanted at a specific position in a SiC crystal.

[1] Simin et al., arXiv:1602.05775v2 (2016)
[2] H. Kraus et al., Nature Phys. **10**, 157 (2014)
[3] F. Fuchs et al., Nature Commun. **6**, 7578 (2015)

TT 82.5 Fri 10:45 POT 81

Three-spin qubits under the influence of tunneling noise — •Maximilian Russ and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We investigate the behavior of qubits consisting of three electron spins in double and triple quantum dots subject to external electric fields[1]. Our model includes two independent bias parameters, ε and ε_M, and two independent tunnel couplings, t_l and t_r, which all couple to external electromagnetic fields and can be controlled in experiments by gate voltages applied to the quantum dot structures. By varying the detuning parameters one can switch the qubit type by shifting the energies in the single quantum dots thus changing the electron occupancy in each dot resulting in different qubit encodings. We focus on random electromagnetic field fluctuations, i.e., "charge noise", at each gate resulting in dephasing of the qubit. We pay special attention to charge noise with respect to the tunnel couplings due to recent interest in symmetric gate operations where the tunnel barrier is controlled. We search for sweet spots and double sweet spots, working points which are least susceptible to noise and compare the results to detuning noise. As a result, we show the absence of non-trivial double sweet spots in the case for tunneling noise.

[1] M. Russ, F. Ginzel, and G. Burkard, Phys. Rev. B 94, 165411 (2016)

TT 82.6 Fri 11:00 POT 81

3-axis magnetometer utilizing silicon vacancy defect spins in 4H silicon carbide — •Matthias Niethammer[1], Matthias Widmann[1], Sang-Yun Lee[1,4], Pontus Stenberg[2], Olof Kordina[2], Takeshi Ohshima[3], Nguyen Tien-Son[2], Erik Janzén[2], and Jörg Wrachtrup[1] — [1]3rd Institute of Physics, University of Stuttgart, IQST and Research Center SCoPE — [2]Department of Physics, Chemistry and Biology, Linköping University — [3]National Institutes for Quantum and Radiological Science and Technology, Takasaki — [4]Korea Institute of Science and Technology, Seoul

Due to their inherent nature spins are very sensitive to magnetic fields. The Zeeman effect can thus be used to sense magnetic fields. Solid state systems as silicon carbide (SiC) can host defects with high spin states, which can be optically detected such as the silicon vacancy (V_{Si}) in 4H-SiC down to the single level at room temperature [1]. In our previous work we showed that the C_{3V} symmetry of this system together with the spin state of $S=\frac{3}{2}$ allows extraction of the magnetic field strength and polar angle [2,3]. Here we demonstrate that an analytical solution in combination with pulsed spin manipulation techniques can be used to measure the complete magnetic field vector even in a large dynamic range [4]. Combined with electrical readout such approaches can lead to highly sensitive and integrated quantum vector magnetometers [5].

1. Widmann et al, Nat. Mater 14(2), 164-168 (2014) 2. Simin et al, Phys Rev Appl 4(1), 014009 (2015) 3. Lee et al, Phys Rev B 92(11), 115201 (2015) 4. Niethammer et al, Phys Rev Appl 6(3), 034001 (2016) 5. Cochrane et al, Sci. Rep. 6, 37077 (2016)

TT 83: Topological Insulators III (joint session DS, HL, MA, O, TT, organized by HL)

Time: Friday 9:30–12:30 Location: POT 251

TT 83.1 Fri 9:30 POT 251

Time-dependent defects in photonic topological insulators — •Christina Jörg[1], Fabian Letscher[1,2], Michael Fleischhauer[1], and Georg von Freymann[1,3] — [1]Physics Department and Research Center OPTIMAS, University of Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, Kaiserslautern, Germany — [3]Fraunhofer-Institute for Physical Measurement Techniques (IPM), Kaiserslautern, Germany

To model topological insulators by means of classical optics, we fabricate arrays of evanescently coupled waveguides. These waveguides are about 1 μm in diameter at an aspect ratio of 1:500, and helically curved. The inverse of the waveguide array is fabricated via direct laser writing in a negative-tone photoresist. Subsequently the sample is infiltrated with a material of higher refractive index, creating low-loss 3D waveguides. Arranging the waveguides on a honeycomb-lattice, a robust edge mode exists due to topological protection [1]. This means that light moves along the edge unidirectionally, and even walks around defects without backscattering. Here, we discuss defects with time-dependent coupling, i.e., one waveguide with a different helicity than the rest of the waveguides. We examine three kinds of time-dependent defects: a) a straight waveguide, b) a waveguide with opposite helicity, c) a waveguide with same helicity but shifted by half a helix pitch in the z-direction. In all three cases the edge mode moves along the edge regardless of the defect, going partially around the defect and partially through it.

[1] M. C. Rechtsman et al., Nature 496, 196-200 (2013).

TT 83.2 Fri 9:45 POT 251

Aharonov-Bohm-type oscillations in HgTe topological insulator nanowires — •Johannes Ziegler[1], Raphael Kozlovsky[2], Ming-Hao Liu[2], Dmitriy Kozlov[1,3,4], Hubert Maier[1], Ze Don Kvon[3,4], Nikolay Mikhailov[3], Sergey Dvoretsky[3], and Dieter Weiss[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Institut für Theoretische Physik, Universität Regensburg, Germany — [3]A.V. Rzhanov Institue of Semiconductor Physics, Novosibirsk, Russia — [4]Novosibirsk State University, Russia

In topological insulator nanowires, the helical surface states form a conducting cylinder enclosing the bulk. These states give rise to Aharonov-Bohm-type oscillations when a magnetic field is applied along the wire axis [1]. These oscillations, periodic with the flux quantum Φ_0, are predicted to change their phase periodically as a function of the Fermi level E_f. We fabricate nanowires with typical cross sections of 80 x 150 nm using an optimized wet etching process to maintain the high mobility and mean free path. In our experiments, we found, as expected, h/e periodic oscillations as a function of magnetic flux Φ with alternating maxima and minima as a function of E_f for $\Phi/\Phi_0 = 1/2$ and $\Phi/\Phi_0 = 1$. We compare the resulting periodicity with a simple model and electrostatic simulations.

[1] J.H. Bardarson *et al.*, Phys. Rev. L **105**, 156803 (2010)

TT 83.3 Fri 10:00 POT 251

Correlation and current anomalies in helical quantum dots — •Christophe De Beule[1], Niccolò Traverso Ziani[2], Mohammad Zarenia[1], Bart Partoens[1], and Björn Trauzettel[2] — [1]Department of Physics, University of Antwerp, 2020 Antwerp, Belgium — [2]Institute of Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

We investigate the ground-state properties of a quantum dot on the surface of a time-reversal invariant topological insulator. Confinement is realized by ferromagnetic barriers and Coulomb interaction is treated with exact diagonalization. The topological origin of the dot has several consequences: (i) spin polarization increases and the ground state exhibits quantum phase transitions as a function of interaction strength, (ii) the onset of Wigner correlations takes place mainly in one spin channel, and (iii) the ground state is characterized by a persistent current that changes direction as a function of the radius.

We also consider the effect of superconducting correlations on the

properties of the quantum dot. This allows us to analyze the influence of perturbations that violate particle-number conservation on the formation of the Wigner molecule.

TT 83.4 Fri 10:15 POT 251

Double topological surface states in strained alpha-Sn — •Victor Rogalev[1], Tomáš Rauch[2], Markus Scholz[1], Felix Reis[1], Lenart Dudy[1], Andrzej Fleszar[3], Marius-Adrian Husanu[4], Vladimir Strocov[4], Jürgen Henk[2], Ingrid Mertig[2,5], Jörg Schäfer[1], and Ralph Claessen[1] — [1]Physikalisches Institut und Röntgen Center for Complex Materials Systems, Universität Würzburg, 97074 Würzburg, Germany — [2]Institute of Physics, Martin Luther University Halle-Wittenberg, 06099 Halle (Saale), Germany — [3]Institut für Theoretische Physik und Astronomie, Universität Würzburg, 97074 Würzburg, Germany — [4]Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen, Switzerland — [5]Max Planck Institute for Microstructure Physics, 06120 Halle (Saale), Germany

The low temperature phase of Sn, α-Sn, is a semimetal with two pairs of "inverted" bands and zero energy band gap, which can be increased by strain. Experimental works revealed so far only one topological surface state (TSS) that bridges one pair of inverted bands.

By means of a combined experimental and theoretical approach we show that the electronic structure of the compressively strained α-Sn (001) thin film hosts an additional TSS in the valence band due to the second band inversion. This sub-surface localized TSS is directly accessed by soft X-ray angle-resolved photoemission with high probing depth. The second TSS reveals a much stronger hybridization with bulk states, in contrast to the already known surface-localized TSS. We show that such difference is consistent with the analysis of orbital composition of bulk and surface states.

TT 83.5 Fri 10:30 POT 251

Stencil lithography of MBE grown superconductors on top of topological insulator thin films — •Michael Schleenvoigt, Peter Schüffelgen, Daniel Rosenbach, Tobias W. Schmitt, Martin Lanius, Benjamin Bennemann, Stefan Trellenkamp, Elmar Neumann, Gregor Mussler, Thomas Schäpers, and Detlev Grützmacher — Peter Grünberg Institute 9, Forschungszentrum Jülich & JARA-FIT, 52425 Jülich, Germany

A stack of the two binary 3D topological insulators Bi2Te3 (n-type doped) and Sb2Te3 (p-type) forms a PN-heterostructure. Growing those topological heterostructures by means of MBE offers the possibility to tune the Fermi level of the upper surface to the Dirac-point. To protect the delicate Dirac system from degradation and oxidation we cap our heterostructures with a thin Al layer, before taking the sample to ambient conditions. We further developed this process to allow for in-situ growth of two different Al layers, i.e. a thin 1-2 nm Al layer on the full wafer followed by a thick Al film on well-defined areas by means of stencil lithography. The thin Al layer will subsequently oxidize after exposure to air and protect the delicate topological surface, whereas the thick Al layer with spatial extent in the (sub-)micrometer range will serve as superconducting contacts. Superconductor-Topological Insulator-Superconductor junctions with lateral dimensions in the nm range have then been fabricated. Despite the in-situ deposition, transport measurements and transmission electron microscope analysis indicate a low transparency, due to an intermixed region at the interface between topological insulator thin film and metallic Al.

Coffee Break

TT 83.6 Fri 11:15 POT 251

Induced superconductivity in lateral topological Josephson junctions with $(Sb_{0.94}Bi_{0.06})_2Te_3$ interlayer — •Daniel Rosenbach[1], Peter Schüffelgen[1], Martin Lanius[1], Gregor Mussler[1], Stefan Trellenkamp[1], Martin P. Stehno[2], Alexander Brinkman[2], Detlev Grützmacher[1], and Thomas Schäpers[1] — [1]Peter Grünberg Institute 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands

The long sought Majorana fermion is predicted to arise in superconducting systems with p-wave pair correlation symmetry. Induced superconductivity in topological insulator thin films is expected to show partly p-wave pairing, such that Majorana zero modes (MZM) are thought to exist at the interface with a conventional s-wave superconductor. A current carried by these zero modes is supposed to show a doubled periodicity in the current-phase relation, compared to conventional modes.

Molecular beam grown topological insulator ternary alloy thin films, of given composition, with a thin aluminum-oxide capping layer, have been prepared with lateral niobium superconducting contacts. Junctions of various geometries have been measured at low temperatures. The response to an externally applied magnetic field and to a radio-frequency signal is strongly dependent on the current-phase relation of the conductive modes. Characterization therefore includes an analysis of various Fraunhofer diffraction pattern as well as Shapiro step measurements at different frequencies.

TT 83.7 Fri 11:30 POT 251

Nontrivial topological phases in quantum mechanical many-body systems with gain and loss effects — •Marcel Klett, Holger Cartarius, and Guenter Wunner — 1. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart

Non-Hermitian $\mathcal{PT}$-symmetric potentials are capable of effectively describing quantum systems with balanced in- and outfluxes. They allow for the existence of a $\mathcal{PT}$-symmetric phase with purely real energy spectra of the non-Hermitian Hamiltonian. Recently a possible relation between the appearance of the $\mathcal{PT}$-symmetric phase and topologically nontrivial states were found in two studies of simple model systems. However, they came to opposite conclusions. In the Su-Schrieffer-Heeger (SSH) model [1] the topological phase has a major influence. As soon as topologically nontrivial states appear $\mathcal{PT}$ symmetry gets broken. This is in contrast to the non-Hermitian Kitaev model [2], in which $\mathcal{PT}$ symmetry breaking does not depend on the topological phase. Our work is based on including different non-Hermitian potentials in the SSH model as well as the Kitaev model. We perform exact calculations of the eigenvalues and the eigenstates, clarify the relation between $\mathcal{PT}$ symmetry and topological phases, and explain why opposite results were found in the above mentioned systems.

[1] Baogang Zhu et al., Phys. Rev. A **89**, 062102 (2014)*
[2] Xiaohui Wang et al., Phys. Rev. A **92**, 012116 (2015)

TT 83.8 Fri 11:45 POT 251

Probing topological edge states in HgTe-based quantum wells by terahertz photogalvanic spectroscopy — •Kathrin-Maria Dantscher[1], Dimitry A. Kozlov[2], Maria-Theresia Scherr[1], Sebastian Gebert[1], Jan Bärenfänger[1], Mikhail Durnev[3], Sergey A. Tarasenko[3], Vasily V. Bel'kov[3], Nikolay N. Mikhailov[2], Sergey A. Dovertsky[2], Ze Dong Kvon[2], Dieter Weiss[1], and Sergey D. Ganichev[1] — [1]Terahertz Center, University of Regensburg, Regensburg, Germany — [2]A.V. Rzhanov Institute of Semiconductor Physics, Novosibirsk 630090, Russia — [3]Ioffe Institute, St.Petersburg, Russia

We report on the observation of a chiral photogalvanic current excited by terahertz laser radiation in the edge channels of HgTe-based 2D topological insulators (TI). The direction of the edge photocurrent reverses by switching the radiation polarization from the right- to left-handed one and, for fixed helicity, has opposite direction for opposite edges. The chiral edge photocurrent is detected in a wide range of gate voltages and reverse the sign twice upon variation of the gate voltage. We show that the data reveal that in the TI-regime the photocurrent is caused by photoionization of helical edge electrons to the conduction band, discuss the microscopic model of this phenomena and present the developed microscopic theory.

TT 83.9 Fri 12:00 POT 251

Topological phase space study of a generalized Kane-Mele spin-orbit Hamiltonian — •Tobias Frank, Petra Högl, Martin Gmitra, Denis Kochan, and Jaroslav Fabian — Theoretische Physik, Universität Regensburg

We study a generalized Kane-Mele [1] graphene spin-orbit coupling Hamiltonian, that is able to describe hybrid systems like graphene on transition metal dichalcogenides [2] or graphene - metal interfaces [3] with broken inversion symmetry. We identify the topological phase space in terms of its Z_2 invariant by variation of spin-orbit coupling parameters. We as well analyze the bulk-edge correspondence in terms of zigzag and armchair ribbons. We find that spin-orbit coupling proximitized graphene can exhibit helical edge states at the zigzag boundary even if it is in the trivial topological phase.

This work is supported by the DFG GRK 1570, SFB 689, and European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

[1] C. L. Kane and E. J. Mele, PRL 95 226801 (2005)
[2] M. Gmitra, D. Kochan, P. Högl, and J. Fabian, PRB 93 155104

(2016)
[3] T. Frank, M. Gmitra, and J. Fabian, PRB 93 155142 (2016)

TT 83.10 Fri 12:15 POT 251

HgTe shells on CdTe nanowires — •Jan Hajer, Maximilian Kessel, Christoph Brüne, Hartmut Buhmann, and Laurens W. Molenkamp — Physikalisches Institut, EP3, Am Hubland, 97074 Würzburg

Topological insulator nanowires in proximity to a superconductor are in research focus of condensed matter physics. Hosting Dirac-like surface states with high spin-orbit coupling, they are a possible platform for p-wave superconductivity and Majorana bound states.

In our work we investigate low temperature charge transport in quasi one-dimensional HgTe. Vapor-liquid-solid grown CdTe nanowires of high crystal quality serve as a substrate for epitaxial HgTe overgrowth. The core-shell heterostructures show residual strain, expected to transform the semi-metallic HgTe shell to a quasi one-dimensional topological insulator. Charge transport with proximitized superconductors indicates a high interface quality giving rise to the observation of multiple Andreev reflections and an induced supercurrent.

TT 84: SYES: Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond (joint symposium DS, HL, MA, MM, O, TT, organized by O)

Time: Friday 10:30–13:00 Location: HSZ 02

Invited Talk TT 84.1 Fri 10:30 HSZ 02

Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations — •Weitao Yang — Duke University

Fractional fractional charges and fractional spins provide a clear analysis of the errors of commonly used functionals. We developed a scaling correction scheme by imposing the Perdew-Parr-Levy- Balduz linearity condition. Our novel scheme leads to the significantly improved description of dissociating molecules, transition-state species, and charge-transfer systems. Within many-electron theory, we have formulated the ground-state exchange-correlation energy in terms of pairing matrix linear fluctuations, opening new a channel for density functional approximations. This method has many highly desirable properties. It has minimal delocalization error with a nearly linear energy behavior for systems with fractional charges, describes van der Waals interactions similarly and thermodynamic properties significantly better than the conventional RPA, and captures the energy derivative discontinuity in strongly correlated systems. We also adopted pp-RPA to approximate the pairing matrix fluctuation and then determine excitation energies by the differences of two-electron addition/removal energies. This approach captures all types of interesting excitations: single and double excitations are described accurately, Rydberg excitations are in good agreement with experimental data and CT excitations display correct 1/R dependence.

Invited Talk TT 84.2 Fri 11:00 HSZ 02

Multi-reference density functional theory — •Andreas Savin — Laboratoire de Chimie Théorique, CNRS and UPMC, Univ. Paris VI, Sorbonne University, Paris, France

It is sometimes said that there is no multi-reference density functional theory. The talk presents a personal viewpoint, and will focus on the following points. 1) There are many ways to introduce multi-determinant wave functions into density functional theory. 2) Several variants have been successfully explored. 3) Difficulties inherent to approximations (both for wave functions and density functionals) persist, but can be attenuated.

Invited Talk TT 84.3 Fri 11:30 HSZ 02

Density functionals from machine learning — •Kieron Burke — UC Irvine

Machine learning is spreading to all aspects of our lives. A particular method, kernel ridge regression, has proven very useful for fitting and interpolating in high-dimensional spaces.

Several years ago, in collaboration with the group of Klaus-Robert Muller in computer science at TU Berlin, we demonstrated how to construct a machine-learned density functional on a simple toy problem, non-interacting fermions in a box. We showed both its successes and limitations. We have continued to develop this method (PRL, 2012).

I will report on two recent works. In the first (arXiv:1609.02815), we construct the non-interacting kinetic energy functional for small molecules in 3D using a basis. We avoid the challenge of finding functional derivatives by learning the potential to density map directly, thereby bypassing the need to solve the Kohn-Sham equations.

In the second, we learn the interacting functional directly for the first time. In 1D, we model chains of H atoms of different length, and learn F[n] itself, from highly accurate DMRG calculations. With a novel choice of basis for the densities, we are able to learn the functional to chemical accuracy in the thermodynamic limit (arXiv:1609.03705).

Invited Talk TT 84.4 Fri 12:00 HSZ 02

Taming Memory-Dependence in Time-Dependent Density Functional Theory — •Neepa Maitra — Hunter College of the City University of New York

The exact exchange-correlation functional of time-dependent density functional theory (TDDFT) is known to depend on the history of the densities and the initial states, a dependence which is ignored in almost all of the calculations today that use an adiabatic approximation. The lack of this dependence can sometimes lead to drastically incorrect predictions of the dynamics, as has been shown in several examples recently. We present here a new approach to developing functional approximations that breaks free of the adiabatic approximation, and test the resulting approximations on a number of model systems.

Invited Talk TT 84.5 Fri 12:30 HSZ 02

Quantum Embedding Theories — •Fred Manby — School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, UK

Issues of accuracy in density functional theory can be addressed by making more accurate methods (like coupled-cluster theory) more efficient; or by making density functional approximations more accurate. Efforts in both directions are underway in our group, but in this talk I will focus on a third possibility, namely the development of quantum-mechnical multiscale models that enable the use of a high-accuracy method in a small, physically important region coupled to density-functional theory (or other low-cost methods) to describe the molecular environment.

TT 85: Graphene: Adsorption, Intercalation and Other Aspects (joint session DY, DS, HL, MA, O, TT, organized by O)

Time: Friday 10:30–13:00 Location: TRE Ma

TT 85.1 Fri 10:30 TRE Ma

Radiation reduced CNM formation from halogenated biphenylthiols — •Sascha Koch[1], Christoph D. Kaiser[1], Lena Frommeyer[1], Patrick Stohmann[1], Tarek Abu-Husein[2], Andreas Terfort[2], and Armin Gölzhäuser[1] — [1]Department of Physics, Universität Bielefeld, Universitätsstrasse 25, 33615 Bielefeld, Germany — [2]Department of Chemistry, Goethe-Universität Frankfurt, Max-von-Laue-Straße 7, 60438 Frankfurt, Germany

Carbon Nano Membranes (CNM) are mechanical stable and homogeneous quasi 2D systems which are formed by the electron radiation induced cross linking of molecules in specific self-assembled monolayers (SAM) grown on substrates like e.g. gold or copper. Contrary to graphene, as the most popular 2D system, the CNM structural and functional properties can be tailored by the selection and composition of appropriate precursors for the SAM formation as for instance phenylthiols or naphthalenes [1,2]. Here, the study of SAMs from halogenated biphenylthiols on a Au(111) substrate is presented. These precursor molecules allow in contrast to hydrogenated biphenylthiols the cross linking of SAMs for the formation of a CNM at a highly reduced electron doses. Additionally, this specific doping of biphenyls provides an insight to the mechanisms of the formation of CNMs. [1] P. Angelova et al., ACS Nano, 2013, 7, 6489-6497 [2] A. Turchanin and A. Gölzhäuser, Adv. Mat. 2016, 28 6075-6103

TT 85.2 Fri 10:45 TRE Ma

Graphene/Polymer Composite Membranes for Nano- and Ultrafiltration — •Lukas Madauss[1], Jens Schumacher[2], Oliver Ochedowski[1], Jens Meyer[2], Henning Lebius[3], Brigitte Band-d'Etat[3], Eugenia Toimil Molares[4], Christina Trautmann[4], Mathias Ulbricht[2], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, Duisburg, Germany — [2]Universität Duisburg-Essen, Essen, Germany — [3]CIMAP, Caen, France — [4]GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, Germany

Nanoporous graphene is currently investigated as a promising membrane material in which selective pores can be created depending on the requirements of the application [1]. Here, we report on the irradiation of nanoporous graphene/polymer composite membranes with swift heavy ions and consecutive track etching. The ions directly create atomic pores in the graphene lattice while cylindrical tracks consisting of damaged material are created in the polymer support. Chemical etching converts the ion tracks in the polymer into large open channels [2] without attacking the graphene layer. The graphene coverage is significantly improved by protecting graphene by a PMMA layer during the track etching process. Our method presents a facile route to create high-quality suspended graphene on a flexible polymeric membrane with pores of tunable size. The development of porous graphene/polymer composite membranes is promising for fast and selective ultrafiltration separation processes.

[1] S. P. Surwade, Nature Nanotechnology, 10, 459-464, 2015 [2] T.W. Cornelius, NIMB, 265, 553-557, 2007

TT 85.3 Fri 11:00 TRE Ma

Optically switchable hybrid graphene/carbon nanomembrane field effect transistors — •Antony George, Zian Tang, David Kaiser, Christof Neumann, Andreas Winter, and Andrey Turchanin — Friedrich Schiller University Jena, Institute of Physical Chemistry, D-07743 Jena, Germany

Field effect transistors (FETs) based on 2D materials are of great interest for applications in ultrathin electronic devices and especially for sensing technology. Here we demonstrate the possibility to add an optical switchability to graphene devices by hybridizing the graphene channel with optically active azobenzene molecules. The azobenzene molecules have been incorporated to the graphene FET channel by building a van der Waals heterostructure with chemically functionalizable 1 nm thin carbon nanomembranes (CNM). Under exposure with 365 nm and 455 nm light azobenzene molecules undergo -cis and-trans molecular conformations resulting in switching of the molecular dipole. We show that these transformations triggered by external optical stimulation induces switching of the graphene FETs between two operation modes.

TT 85.4 Fri 11:15 TRE Ma

Insight into the wetting of a graphene-mica slit pore with a monolayer of water — •Hu Lin, Andre Schilo, Rauf Kamoka, Nikolai Severin, Igor M. Sokolov, and Jürgen P. Rabe — Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Graphene-mica slit pores are prepared by mechanical exfoliation of graphite onto a freshly cleaved muscovite mica surface in dry nitrogen. We followed their wetting and dewetting with water by scanning force microscopy (SFM) and Raman spectroscopy, which allows to unravel doping and strain effects upon both wetting and dewetting. SFM reveals that the wetting water layer is one monolayer thick, slightly thinner than a single layer of graphene. Raman spectra exhibit a reduction of the graphene D' peak intensity upon wetting, and a recurrence of the peak when the water layer dewets the slit pore. We attribute the D' peak to direct contact of the graphene with the ionic mica surface in dry conditions. Analyses of the 2D and G peak positions, the corresponding peak positions and the widths, imply that graphene on dry mica is charge doped and variably strained. A monolayer of water in between graphene and mica removes doping and reduces strains. This supports that in dry conditions graphene is in direct contact with the mica surface, while a complete monolayer of water wetting the slit pore decouples the graphene from the mica substrate both mechanically and electronically.

TT 85.5 Fri 11:30 TRE Ma

Substrate topography and annealing of Co/Gr/SiC(0001) investigated by means of photoemission electron microscopy — •Richard Hönig, Philipp Espeter, Peter Roese, Karim Shamout, Hermann Kromer, Ulf Berges, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4a, 44227 Dortmund, Germany

The realization of carbon electronics requires semiconducting substrates, therefore epitaxial graphene on silicon carbide is a promising candidate. Challenges with this system are the covalently bonded buffer layer impacting the electronic properties, and the limited graphene grain size depending on the preparation conditions.

Here, the so-called confinement controlled sublimation is applied to yield a high grain size. The characterization of the samples has been carried out by photoemission electron microscopy (PEEM) which combines surface sensitivity with a mesoscopic resolution and unique contrast mechanisms. Images of samples prepared under high vacuum or under inert gas conditions are presented.

In order to decouple the buffer layer as well as for tailoring the properties of this multilayer system, the intercalation of metals underneath graphene is a common method. Consequently, we will present the first attempts of cobalt intercalation.

TT 85.6 Fri 11:45 TRE Ma

Oxygen intercalation at the graphene/Ni(111) interface — •Luca Bignardi[1], Paolo Lacovig[1], Matteo Dalmiglio[1], Fabrizio Orlando[1,2], Aliakbar Ghafari[1,3], Luca Petaccia[1], Alessandro Baraldi[1,4], Rosanna Larciprete[5], and Silvano Lizzit[1] — [1]Elettra - Sincrotrone Trieste, Trieste, Italy — [2]Paul Scherrer Institut - Villingen PSI, Switzerland — [3]Helmholtz-Zentrum Berlin, Berlin, Germany — [4]Università degli Studi di Trieste, Trieste, Italy — [5]CNR - Istituto dei Sistemi Complessi, Rome, Italy

Intercalation of atomic species at the graphene-substrate interface is an effective way to decouple graphene (GR) from the metal on which it is grown, restoring the Dirac cone and tuning the GR-substrate interaction. The intercalation of oxygen was found to be successful, independently of the extent of the graphene-metal interaction, upon a suitable choice of oxygen partial pressure and sample temperature. Herein we report on the intercalation and de-intercalation of oxygen at the strongly interacting Gr/Ni(111) interface. Synchrotron-radiation based high-resolution X-ray photoelectron spectroscopy was used to characterise the intercalation mechanism and the nature of the compounds at the interface. We observed that the intercalated oxygen efficiently decouples the GR layer quenching the hybridisation with the metal substrate. Angle-resolved photoelectron spectroscopy measurements showed the restoration of the Dirac cone band-structure.

Moreover, X-ray photoelectron diffraction added further insight into the structure of GR in the different phases of the process.

TT 85.7 Fri 12:00 TRE Ma

Graphene phonons in inelastic electron tunnelling spectroscopy — •Johannes Halle[1], Nicolas Néel[1], Mads Brandbyge[2], and Jörg Kröger[1] — [1]Technische Universität Ilmenau, Ilmenau, Germany — [2]Technical University of Denmark, Lyngby, Denmark

Graphene on Ir(111) was intercalated by Li, Cs, and Ni. Inelastic electron tunnelling spectroscopy (IETS) unraveled remarkably strong signatures of graphene phonons for Li and Cs intercalants. For Ni-intercalated graphene, in contrast, phonon signals stayed below the detection limit of the low-temperature scanning tunnelling microscope (STM). On the basis of previously determined phonon dispersion branches the IETS features were assigned to acoustic and optical graphene phonons at the M point of the surface Brillouin zone. Additional experiments unveiled that the IETS signal increased with increasing Li coverage. Moreover, decreasing the separation between STM tip and graphene from the tunnelling to contact ranges led to a significant lowering of the phonon spectroscopic signatures. Combining these results, and comparing to transport calculations based on density functional theory, we discuss possible mechanisms that appropriately describe inelastic excitations with non-zero wave vectors via electron injection from an STM tip. Financial support by the Deutsche Forschungsgemeinschaft through Grant No. KR 2912/10-1 is acknowledged.

TT 85.8 Fri 12:15 TRE Ma

Electronic transport properties of novel nanosensors based on graphene and beyond — •Frank C. Maier[1], Ganesh Sivaraman[1], Fabio A.L. de Souza[2], Rodrigo G. Amorim[3], Wanderla L. Scopel[2], Ralph H. Scheicher[4], and Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Departamento de Fisica, Universidade Federal do Espirito Santo, Vitoria/ES, Brazil — [3]Universidade Federal Fluminense, Departamento de Física, Volta Redonda/RJ, Brazil — [4]Department of Physics and Astronomy, Materials Theory, Uppsala University, Sweden

In this work, we investigate the sensing abilities of graphene based-materials. Specifically, we focus of pristine graphene and on a hybrid graphene/hexagonal boron nitride monolayer. Using density functional theory based simulations together with the non-equilibrium Green's functions formalism we are able to calculate the electronic transport across these materials, which serve as a reference. At a next step we choose small molecules (such as NO2, CO2, H2S, benzene derivatives, etc.) and attach these covalently and/or non-covalently on the graphene materials. We first analyze the structural and electronic properties of these modified graphene-based monolayers and the molecule specific signatures. Our aim is to predict their electronic transport properties and evaluate the change in the properties and the charge transfer with respect to the type of the attached molecule. In the end, we discuss our results in view of using graphene-based sensors for label-free detection of molecules and binding events.

TT 85.9 Fri 12:30 TRE Ma

Switching the reactivity of graphene on Ir(111) by hydrogen intercalation. — •Richard Balog[1], Andrew Cassidy[1], Line Kyhl[1], Jakob Jorgensen[1], Antonia Cabo[1], Luca Bignardi[1], Paolo Lacovig[2], Silvano Lizzit[2], Philip Hofmann[1], and Liv Hornekaer[1] — [1]Department of Physics and Astronomy and Interdisciplinary Nanoscience Center iNANO, Aarhus University, Aarhus C DK-8000, Denmark — [2]Elettra-Sincrotrone Trieste S.C.p.A., S.S. 14 Km 163.5, 34149 Trieste, Italy

In this paper I will present XPS and STM data revealing the modified reactivity of graphene towards hydrogen when intercalated. First I will show that the extent of hydrogen intercalation can be monitored by the progressive downshift of C1s spectra until fully decoupled a quasi-freestanding graphene is formed on Ir(111). Secondly, I will show that this intercalation affects the reactivity of graphene towards H atoms but also vibrationally excited H2 molecules. I will show that while graphene on Ir(111) can be functionalized upon exposure to vibrationally excited H2, the reactions is fully suppressed in a quasi-freestanding state. Controlling the reactivity of graphene towards outer environment simply by modification of its interaction with an underlying substrate paves the way for future application of (functionalized) graphene in everyday devices.

TT 85.10 Fri 12:45 TRE Ma

Intercalation and Deintercalation of Lithium at the Ionic Liquid|Graphite(0001) Interface — •Florian Buchner[1], Jihyun Kim[2], Christiane Adler[2], Joachim Bansmann[2], and R. Jürgen Behm[1,2] — [1]Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89081 Ulm, Germany — [2]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

The intercalation and deintercalation of lithium (Li) on the graphite anode in Li-ion batteries is essential for their function. This was investigated in a model study under ultrahigh vacuum conditions as a function of temperature employing X-ray and UV photoelectron spectroscopy (XPS / UPS). After vapor deposition of metallic Li, partially charged $Li^{\delta+}$ atoms were identified on graphite(0001) at 80 K, while, they diffuse into the bulk at 300 K. Interestingly, the ionic liquid (IL) 1-butyl-1-methyl-pyrrolidinium bis-(trifluoromethylsulfonyl)amide [BMP][TFSA], which is a promising solvent/electrolyte, can be used as a probe to measure $Li^{\delta+}$ deintercalation. After adsorption of a [BMP][TFSA] (sub-)monolayer on lithiated graphite at 80 K, the sample was heated to 300 K. Both the gradual shifts of all adsorbate-related XP peaks at > 230 K and the simultaneous lowering of the work function indicate the accumulation of partially charged $Li^{\delta+}$ atoms at the IL|graphite(0001) interface. This is accompanied by a partial decomposition of the IL adlayer (LiF, Li_2S, and LiN_3, etc.), which we associate with the initial stages of the chemical formation of the electrode|electrolyte interface (EEI), which in turn is crucial for the function of batteries.

TT 86: Low-Dimensional Systems: Charge Order

Time: Friday 11:15–12:00 Location: HSZ 103

TT 86.1 Fri 11:15 HSZ 103

Origin of the negative plasmon dispersion in $NbSe_2$ and related systems. — •Eric Müller, Martin Knupfer, and Bernd Büchner — IFW-Dresden, P.O.Box 270116, DE-01171 Dresden, Germany

The charge carrier plasmon excitations of $2H$-$NbSe_2$ 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 compare two possible routes to explain the observed unusual negativ plasmon dispersion; charge density wave plasmon interaction and band structure effects. Motivated by the orbital character of the plasmon dispersion in alkali metal doped transition metal dichalcogenides, we demonstrate that the separation of the plasmon from the screening contributions of single particle excitations by a Kramers-Kronig analysis reveals a positive (unscreened) plasmon dispersion.

TT 86.2 Fri 11:30 HSZ 103

Electronic self-organization in layered transition metal dichalcogenides — •Tobias Ritschel[1], Jan Trinckauf[2], Martin von Zimmermann[3], Klaus Koepernik[2], Peter Abbamonte[5], Young Joe[5], Helmuth Berger[4], Bernd Büchner[1,2], and Jochen Geck[1] — [1]TU Dresden — [2]IFW, Dresden — [3]DESY Hamburg — [4]Ecole polytechnique Federale de Lausanne — [5]University of Illinois

We combined density functional theory (DFT) with angle-resolved photoemission spectroscopy (ARPES) and x-ray diffraction to discover that the electronic order in the prototypical charge density wave system 1T-TaS_2 involves complex orbital textures. Most importantly, the low energy electronic band structure parallel to the layers depends crucially on the stacking of these orbital textures in the perpendicular direction, which challenges the classical view of these materials as being quasi 2D-systems. Recently, we refined our DFT models to implement an approximation of the partially disordered character, which is found experimentally for the orbital texture stacking in the so-called Mott-phase of 1T-TaS_2. The excellent agreement of these simulations

with ARPES data indicates that the previous paradigm of a Mott-gap in this system needs to be reconsidered. Instead, we find firm evidence that the corresponding gap is predominantly caused by hybridization between the orbital textures in adjacent TaS_2-layers. We will discuss these results with respect to recent experiments which reported marked changes of macroscopic properties in exfoliated transition metal dichalcogenides as a function of thickness. Understanding such effects is increasingly important with respect to future applications.

TT 86.3 Fri 11:45 HSZ 103

Pressure dependent x-ray diffraction study of the electronic order in $IrTe_2$ — •Maximilian Kusch[1,2], Tobias Ritschel[2], Jan Trinckauf[1], Gaston Garbarino[3], Sang-Wook Cheong[4], and Jochen Geck[2] — [1]Institute for Solid State and Materials Research, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Institut für Strukturphysik, Technische Universität Dresden D-01062 Dresden, Germany — [3]European Synchrotron Radiation Facility, B.P.220, 38043 Grenoble, France — [4]Department of Physics and Astronomy Rutgers, The State University of New Jersey 136 Frelinghuysen Road Piscataway, NJ 08854-8019 USA

The proximity of spatial electronic order and superconductivity in the transition metal dichalcogenides (TMDs) currently attracts a lot of interest. At ambient pressure, also pristine IrTe2 exhibits electronic order below $T_s \approx 250$ K and becomes superconducting upon doping with Pd and Pt, although it remains unclear whether this transition is similar to other TMDs. In addition, contrary to other TMDs, measurements of the electrical resistivity indicate a stabilization of the electronic order accompanied by a suppression of the superconducting phase. In order to clarify the underlying physics we performed pressure dependent single crystal XRD measurements up to 42 GPa on $IrTe_2$ and its Pd (4%) and Pt (7%) doped variants. Our data reveal two transitions in $IrTe_2$ upon increasing pressure, where the first one is identified by surprisingly strong superlattice reflections, whereas the second one is better described by a transformation into a completely new crystal structure with a large unit cell.

TT 87: Optics and Light-Matter Interaction with Excitons in 2D Materials (joint session HL, DS, O, and TT, organized by DS)

Time: Friday 11:15–12:15 Location: CHE 89

TT 87.1 Fri 11:15 CHE 89

Enhanced light-matter interaction in graphene/h-BN van der Waals heterostructures — •Caterina Cocchi[1], Wahib Aggoune[1,2], Dmitrii Nabok[1], Karim Rezouali[2], Mohamed Akli Belkhir[2], and Claudia Draxl[1,2] — [1]Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Laboratoire de Physique Théorique, Faculté des sciences exactes, Université de Bejaia, 06000 Bejaia, Algeria

Investigating the electronic and optical properties of graphene/h-BN heterostructures from first principles, we observe a peculiar nature of their excitations. To this extent, we employ density-functional and many-body perturbation theory in terms of the GW approximation and the Bethe-Salpeter equation. The interaction with h-BN opens a gap in graphene, making the heterostructures semiconducting. These systems absorb light over a broad frequency range, from the near-infrared to the ultraviolet region, exhibiting novel features induced by the stacking. While the specific properties of the building blocks are basically preserved, the inter-layer electron-hole pairs that are formed in the heterostructure can be modulated upon layer patterning. By choosing the stacking arrangement, the electronic coupling between the individual components can be tuned to enhance light-matter interaction. Our results open up perspectives in view of designing new low-dimensional materials with tailored opto-electronic characteristics.

TT 87.2 Fri 11:30 CHE 89

Spectral Focusing of Broadband Silver Electroluminescence in Nanoscopic FRET-LEDs — •Robin Puchert, Florian Steiner, Gerd Plechinger, Felix Hofmann, Christian Schüller, Tobias Korn, Jan Vogelsang, Sebastian Bange, and John Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Universitätsstrasse 31, 93053 Regensburg, Germany

A challenge in LED technology is the use of fluorescence resonance energy transfer (FRET) in spectral conversion. An LED based on FRET effect would show both up- and down-conversion of electroluminescence (EL), since the electrically driven resonance of the light emitting device (donor) couples non-radiatively to the acceptor fluorophore resonance.

FRET-LEDs have already been proposed. However, such devices have yet to be demonstrated. The challenge lies in generating light electrically in close proximity to a dipolar acceptor in order to allow near-field coupling. We present a solution to this problem by combining a lateral LED structure with a two-dimensional transition-metal dichalcogenide overlayer (TMDC). The LED's entire excitation energy is transferred to the 2D crystal overlayer through resonant dipole-dipole coupling rather than by trivial reabsorption. This is quite remarkable given the fact that such an atomically thin TMDC monolayer absorbs only a mere 4 % of light. By using plasmonic silver nanoparticle junctions to generate broad-band EL coming from sub-diffraction localized hotspots, we see dramatic spectral focusing of the EL into the narrow excitonic resonance of the atomically thin overlayer.

TT 87.3 Fri 11:45 CHE 89

Spin-flip transitions induced by time-dependent electric fields in tuned Transition Metal Dichalcogenides magnetic thin films. — •Omar Messaoudi[1,2], Julen Ibañez-Azpiroz[2], Hamid Bouzar[1], and Samir Lounis[2] — [1]Université Mouloud Mammeri de Tizi Ouzou, Tizi Ouzou, Algeria — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

We study from first principles the relativistic electron structure of Transition Metal Dichalcogenides such as MoS_2 and WS_2 on top of which Iron is deposited as a monolayer or as a single impurity. The resulting systems turn out to be magnetic and, in particular, the states near the Fermi level show a non-negligible noncollinear spin-polarization due to the effect of spin-orbit coupling. In these noncollinear states, we analyze the excitations induced by a time-dependent electric field employing a formalism based on the maximally localized Wannier functions [1]. Finally, we analyze the absorption spectrum of circularly polarized light and discuss the possibility of observing a dichroic signal.

[1] J. Ibañez-Azpiroz *et. al*, Phys. Rev. Lett. **109**, 156401 (2012)

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TT 87.4 Fri 12:00 CHE 89

Ab-initio calculations of valley depolarization in single-layer WSe_2 mediated by electron-phonon interaction — Alejandro Molina-Sánchez[1], Davide Sangalli[2], Andrea Marini[2], and •Ludger Wirtz[1] — [1]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [2]Istituto de Strutura della Materia (CNR), CNR, Monterrotondo, Rome, Italy

Circularly polarized light can be used to selectively populate the K^+ and K^- electronic valleys of single-layer WSe_2. Valley depolarization has been measured through time-dependent Kerr experiments (measuring the rotation of a linearly polarized probe pulse applied after a circularly polarized pump pulse) by several groups. However, the depolarization mechanism still remains largely debated. Using an ab-initio implementation of time-dependent many-body perturbation theory (including electron-electron, electron-hole, and electron-phonon interaction), we solve unambiguously the debate about the dominant mechanism that drives the valley depolarization. The decay dynamics and peculiar temperature dependence (observed in recent experiments) is explained in terms of electron-phonon mediated processes that induce spin-flip inter-valley transitions.