Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

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Overview of Invited Talks and Sessions

(Lecture rooms H18-23; Poster D2)

Tutorials

TT 1.1	Sun	16:00–16:45	H20	**Correlation functions of integrable models** — •Frank Göhmann
TT 1.2	Sun	16:45–17:30	H20	**Non-Abelian anyons** — •Holger Frahm
TT 1.3	Sun	17:45–18:30	H20	**Quantum quenches and equilibration of lattice and continuum systems** — •Michael Brockmann

Invited Talks

TT 5.7	Mon	11:30–12:00	H22	**Coherent Suppression of Quasiparticle Dissipation in a Superconducting Artificial Atom** — •Ioan Pop
TT 14.7	Mon	16:45–17:15	H19	**Spectroscopic signatures of collective modes in superconductors** — •Lara Benfatto
TT 15.1	Mon	15:00–15:30	H20	**Thermodynamics of Fractional Quantum Spin Liquids** — •Yukitoshi Motome
TT 15.2	Mon	15:30–16:00	H20	**Proximate Kitaev quantum spin liquid behavior in α-RuCl$_3$** — •Stephen Nagler
TT 15.3	Mon	16:00–16:30	H20	**Kagome chiral spin liquid and symmetry protected topological phases** — •Yin-Chen He
TT 15.4	Mon	16:45–17:15	H20	**Three-dimensional Kitaev spin liquids** — •Maria Hermanns
TT 15.5	Mon	17:15–17:45	H20	**Landau levels of Majorana fermions in a spin liquid** — •Matthias Vojta
TT 24.1	Tue	9:30–10:00	H18	**Detecting Weyl fermions in condensed matter** — •Titus Neupert
TT 26.1	Tue	9:30–10:00	H20	**Classical and quantum correlation induced bias asymmetries in coupled spin systems** — •Markus Ternes
TT 26.2	Tue	10:00–10:30	H20	**Magnetic anisotropy goes spintronic** — •Maarten R. Wegewijs
TT 26.3	Tue	10:30–11:00	H20	**Engineering the Kondo Effect in clean Carbon Nanotubes** — •Christoph Strunk
TT 26.4	Tue	11:15–11:45	H20	**Majorana Fermions in Atomic Chains** — •Ali Yazdani
TT 26.5	Tue	11:45–12:15	H20	**Magnetic adatoms on superconductors - a new venue for Majorana bound states?** — •Felix von Oppen
TT 30.1	Tue	11:00–11:30	H19	**Selective correlations and heavy-fermionic behaviour in Iron-based superconductors** — •Luca de' Medici
TT 32.1	Tue	14:00–14:30	H18	**Coupled-wire constructions: New insights into the physics of interacting topological systems in two and three dimension (and beyond)** — •Tobias Meng
TT 37.5	Tue	15:00–15:30	H23	**Dynamical Coulomb Blockade theory of resonantly enhanced light emission from a tunnel junction** — •Wolfgang Belzig
TT 43.11	Wed	12:15–12:45	H20	**Rare-earth-like behavior of transition metals substituted in Li$_3$N** — •Anton Jesche
TT 44.1	Wed	9:30–10:00	H22	**Ultrafast photo-thermoelectric currents in graphene** — •Alexander Holleitner
TT 46.6	Wed	11:30–12:00	H19	**On Nematicity, Magnetism and Superconductivity in FeSe** — •A. E. Böhmer

TT 52.1	Wed	15:00–15:30	H20	**Hund's Metals: a New Road to Strongly Correlated Electron Behavior** — •Gabriel Kotliar
TT 52.2	Wed	15:30–16:00	H20	**Screened Exchange Dynamical Mean Field Theory** — •Silke Biermann
TT 52.3	Wed	16:00–16:30	H20	**Dynamical Screening in Correlated Electron Materials** — •Philipp Werner
TT 52.4	Wed	16:45–17:15	H20	**Lattice stability of correlated electron materials** — •Ivan Leonov
TT 52.5	Wed	17:15–17:45	H20	**Tin Foil at the Nanometer Scale - from Electronic Correlations to Topological Physics** — •Ralph Claessen
TT 52.6	Wed	17:45–18:15	H20	**Electron Correlations in Nanosystems and 2D Materials: What's so Different from Bulk?** — •Tim Wehling
TT 54.7	Wed	16:45–17:15	H22	**Cooling a nanomechanical resonator by electron transport in hybrid devices.** — •Gianluca Rastelli
TT 62.1	Thu	9:30–10:00	H20	**Conventional high temperature superconductivity: from A15 to MgB_2 to H_3S** — •Igor Mazin
TT 62.2	Thu	10:00–10:30	H20	**Conventional superconductivity at 203 K at high pressures** — •Mikhail Eremets
TT 62.3	Thu	10:30–11:00	H20	**Crystal Structure of 200 K-Superconducting Phase in Sulfur Hydride System** — •Mari Einaga
TT 62.4	Thu	11:15–11:45	H20	**Strong-Coupling Electron-Phonon Superconductivity in H_3S** — •Warren E. Pickett
TT 62.5	Thu	11:45–12:15	H20	**High-pressure phases of S, Se, and P hydrides and their superconducting properties: Predictions from ab-initio theory** — •E. K. U. Gross
TT 62.6	Thu	12:15–12:45	H20	**New sulfur hydride H_3S and excellent superconductivity at high** — •Tian Cui
TT 73.7	Thu	16:45–17:15	H19	**Imaging currents in 2D quantum materials** — •Katja Nowack
TT 81.1	Thu	16:15–16:45	H23	**Non-Abelian gauge theory description of (dynamical) spin-orbit coupling effects in Fermi gases.** — •Cosimo Gorini

Invited talks of the joint symposium SYTI

See SYTI for the full program of the symposium.

SYTI 1.1	Wed	9:30–10:10	H1	**Topological insulators and topological superconductors** — •Shoucheng Zhang
SYTI 1.2	Wed	10:10–10:50	H1	**Three-dimensional topological insulators and superconductors** — •Yoichi Ando
SYTI 1.3	Wed	10:50–11:30	H1	**Interplay of magnetic and electronic states in pyrochlore iridates** — •Leon Balents
SYTI 1.4	Wed	11:40–12:20	H1	**Magnetic imaging of edge states** — •Kathryn Moler
SYTI 1.5	Wed	12:20–13:00	H1	**Sub-nm wide edge states at the dark side of a weak topological insulator** — •Markus Morgenstern

Invited talks of the joint symposium SYQS

See SYQS for the full program of the symposium.

SYQS 1.1	Wed	15:00–15:30	H1	**Magnonic macroscopic quantum states and supercurrents** — •Burkard Hillebrands, Dmytro A. Bozhko, Alexander A. Serga
SYQS 1.2	Wed	15:30–16:00	H1	**Elementary excitations of magnetic insulators and its heterostructures with metals** — •Gerrit Bauer
SYQS 1.3	Wed	16:00–16:30	H1	**Cavity Spintronics** — •Can-Ming Hu
SYQS 1.4	Wed	16:45–17:15	H1	**Hybrid Quantum Systems - Coupling Color Centers to Superconducting Cavities** — •Johannes Majer
SYQS 1.5	Wed	17:15–17:45	H1	**Quantum enhanced sensing with single spins in diamond** — •Fedor Jelezko

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Intrinsic Transport Coefficients and Momentum Space Berry Curvatures** — •Allan H MacDonald
SYES 1.2	Fri	10:00–10:30	H1	**Berry phase linked spin-orbit torques in Ferromagnetic and Antiferromagnetic systems** — •Jairo Sinova
SYES 1.3	Fri	10:30–11:00	H1	**Transport in Topological Insulators and Topological Superconductors: In Search of Majorana Fermions** — •Ewelina Hankiewicz
SYES 1.4	Fri	11:15–11:45	H1	**Engineering Topological Quantum States: From 1D to 2D.** — •Jelena Klinovaja
SYES 1.5	Fri	11:45–12:15	H1	**Skyrmions – Topological magnetization solitons for future spintronics** — •Stefan Blügel

Sessions

TT 1.1–1.3	Sun	16:00–18:30	H20	**Tutorial: Correlations in Integrable Quantum Many-Body Systems**
TT 2.1–2.10	Mon	9:30–12:30	H17	**Graphene: Theory** **(Joint session of DS, DY, HL, MA, O and TT organized by HL)**
TT 3.1–3.13	Mon	9:30–13:00	H20	**Correlated Electrons: Frustrated Magnets - Pyrochlore Systems and Iridates**
TT 4.1–4.12	Mon	9:30–12:45	H47	**Dynamics in many-body systems: Equilibriation and localization** **(Joint session of DY and TT organized by DY)**
TT 5.1–5.11	Mon	9:45–13:00	H22	**Transport: Quantum Coherence and Quantum Information Systems - Experiment** **(Joint session of HL, MA and TT organized by TT)**
TT 6.1–6.11	Mon	10:00–13:00	H19	**Superconductivity: Properties and Electronic Structure**
TT 7.1–7.10	Mon	10:15–13:00	H18	**Cold Atomic Gases**
TT 8.1–8.10	Mon	10:15–13:00	H21	**Correlated Electrons: Quantum Impurities, Kondo Physics**
TT 9.1–9.11	Mon	10:30–13:30	H24	**Graphene: Structure and Dynamics** **(Joint session of DS, DY, HL, MA, O and TT organized by O)**
TT 10.1–10.4	Mon	11:30–13:00	H10	**Focus Session: Single Particle Sources for Electronic Devices I** **(Joint session of HL and TT organized by HL)**
TT 11.1–11.10	Mon	14:45–18:45	H10	**Focus Session: Single Particle Sources for Electronic Devices II** **(Joint session of HL and TT organized by HL)**
TT 12.1–12.8	Mon	14:45–17:45	H17	**Graphene: Transport** **(Joint session of DS, DY, HL, MA, O and TT organized by HL)**
TT 13.1–13.10	Mon	15:00–17:45	H18	**Transport: Topological Insulators - 2D** **(Joint session of DS, HL, MA, O and TT organized by TT)**
TT 14.1–14.10	Mon	15:00–18:00	H19	**Superconductivity: (General) Theory**
TT 15.1–15.5	Mon	15:00–17:45	H20	**Focus Session: Spectroscopy of Quantum Spin Liquids**
TT 16.1–16.10	Mon	15:00–17:45	H21	**Transport: Quantum Dots, Quantum Wires, Point Contacts**
TT 17.1–17.8	Mon	15:00–17:15	H22	**Low-Dimensional Systems: Oxide Hetero-Interfaces**
TT 18.1–18.12	Mon	15:00–18:15	H31	**Spincaloric Transport** **(Joint session of MA and TT organized by MA)**
TT 19.1–19.56	Mon	15:00–18:00	Poster D	**Superconductivity: Poster Session**
TT 20.1–20.6	Mon	15:00–18:00	Poster D	**Cryotechnique & Measuring Devices: Poster Session**
TT 21.1–21.7	Mon	15:45–17:45	H51	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport** **(Joint session of DS, HL, MA, MM, O and TT organized by MM)**
TT 22.1–22.4	Mon	17:45–18:45	H17	**Graphene: Fabrication** **(Joint session of DS, DY, HL, MA, O and TT organized by HL)**

TT 23.1–23.10	Tue	9:30–12:30	H15	**Quantum Information Systems (Joint session of HL, MA, O and TT organized by HL)**
TT 24.1–24.12	Tue	9:30–13:00	H18	**Transport: Weyl Semimetals**
TT 25.1–25.5	Tue	9:30–10:45	H19	**Superconductivity: Fe-based Superconductors - 1111 & 111**
TT 26.1–26.5	Tue	9:30–12:15	H20	**Focus Session: Engineered Magnetic Impurities: Interaction and Superconductivity**
TT 27.1–27.12	Tue	9:30–12:45	H22	**Transport: Quantum Coherence and Quantum Information Systems - Theory 1 (Joint session of HL, MA and TT organized by TT)**
TT 28.1–28.11	Tue	10:00–13:00	H21	**Correlated Electrons: Quantum-Critical Phenomena - Experiment**
TT 29.1–29.11	Tue	10:30–13:30	S051	**Topology- and Symmetry-Protected Materials (Joint session of DS, HL, MA, O and TT organized by O)**
TT 30.1–30.7	Tue	11:00–13:00	H19	**Superconductivity: Fe-based Superconductors - Theory**
TT 31.1–31.2	Tue	12:30–13:00	H8	**Topological Insulators: Status Quo and Future Directions (Joint session of DS, MA, HL, O and TT organized by DS)**
TT 32.1–32.6	Tue	14:00–15:45	H18	**Transport: Topological Insulators - 3D (Joint session of DS, HL, MA, O and TT organized by TT)**
TT 33.1–33.6	Tue	14:00–15:30	H19	**Superconductivity: Cryodedetectors & Cryotechnique**
TT 34.1–34.8	Tue	14:00–16:00	H20	**Correlated Electrons: Frustrated Magnets - Chiral Magnets & $RuCl_3$**
TT 35.1–35.7	Tue	14:00–15:45	H21	**Correlated Electrons: Quantum-Critical Phenomena - Theory**
TT 36.1–36.4	Tue	14:00–15:00	H22	**Transport: Quantum Coherence and Quantum Information Systems - Theory 2 (Joint session of HL, MA and TT organized by TT)**
TT 37.1–37.6	Tue	14:00–15:45	H23	**Transport: Fluctuation and Noise (Joint session of DY and TT organized by TT)**
TT 38.1–38.7	Tue	14:00–16:00	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport I (Joint session of DS, HL, MA, MM, O and TT organized by O)**
TT 39.1–39.8	Tue	14:00–16:00	S051	**Spintronics (Joint session of DS, HL, MA, O and TT organized by O)**
TT 40.1–40.3	Tue	14:45–15:45	H17	**Graphene: Optics (Joint session of DS, DY, HL, MA, O and TT organized by HL)**
TT 41.1–41.5	Wed	9:30–13:00	H1	**Symposium Topological Insulators: Status Quo and Future Directions (SYTI) (Joint symposium of HL, MA, O and TT organized by TT)**
TT 42.1–42.13	Wed	9:30–13:00	H18	**Correlated Electrons: Frustrated Magnets - Cu-based Systems & FeCr**
TT 43.1–43.12	Wed	9:30–13:00	H20	**Correlated Electrons: f-Electron & Heavy Fermion Systems**
TT 44.1–44.13	Wed	9:30–13:15	H22	**Transport: Graphene (Joint session of DS, DY, HL, MA, O and TT organized by TT)**
TT 45.1–45.10	Wed	9:30–12:15	H32	**Spintronics (incl. Quantum Dynamics) (Joint session of MA, HL and TT organized by MA)**
TT 46.1–46.9	Wed	10:00–12:45	H19	**Superconductivity: Fe-based Superconductors - FeSe**
TT 47.1–47.9	Wed	10:30–13:00	H21	**Correlated Electrons: Other Materials**
TT 48.1–48.10	Wed	10:30–13:00	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport II (Joint session of DS, HL, MA, MM, O and TT organized by O)**
TT 49.1–49.5	Wed	15:00–17:45	H1	**Symposium on Quantum Signatures in Magnetism (SYQS) (Joint symposium of HL, MA, O and TT organized by MA)**
TT 50.1–50.15	Wed	15:00–19:15	H18	**Correlated Electrons: Frustrated Magnets - Theory**
TT 51.1–51.14	Wed	15:00–19:00	H19	**Superconductivity: Tunneling, Josephson Junctions, SQUIDs**
TT 52.1–52.6	Wed	15:00–18:15	H20	**Focus Session: Realistic Dynamical Mean-Field Approaches to Correlated Quantum Materials**
TT 53.1–53.12	Wed	15:00–18:15	H21	**Low-Dimensional Systems: 1D - Theory**
TT 54.1–54.11	Wed	15:00–18:15	H22	**Transport: Carbon Nanotubes**

TT 55.1–55.12	Wed	15:00–18:30	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport III (Joint session of DS, HL, MA, MM, O and TT organized by O)**
TT 56.1–56.12	Wed	15:00–18:00	S053	**Graphene: Adsorption, Intercalation and Doping (Joint session of DS, DY, HL, MA, O and TT organized by O)**
TT 57.1–57.10	Wed	15:00–17:45	H32	**Topological Insulators (Joint session of MA, DS, HL, O and TT organized by MA)**
TT 58.1–58.54	Wed	15:00–18:30	Poster D	**Transport: Poster Session**
TT 59.1–59.22	Wed	15:00–18:30	Poster D	**Low-Dimensional Systems: Poster Session**
TT 60.1–60.7	Wed	18:15–20:30	Poster A	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport (Joint session of DS, HL, MA, MM, O and TT organized by O)**
TT 61.1–61.13	Thu	9:30–13:00	H18	**Correlated Electrons: (General) Theory 1**
TT 62.1–62.6	Thu	9:30–12:45	H20	**Focus Session: High Temperature Superconductivity in Hydrides**
TT 63.1–63.13	Thu	9:30–13:00	H21	**Low-Dimensional Systems: 2D - Theory**
TT 64.1–64.13	Thu	9:30–13:00	H22	**Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 1**
TT 65.1–65.13	Thu	9:30–13:00	H23	**Transport: Molecular Electronics and Photonics 1 (Joint session of CPP, DS, HL, MA, O and TT organized by TT)**
TT 66.1–66.11	Thu	9:30–12:30	H34	**Magnetic Heusler Materials, Semimetals und Oxides (Joint session of MA and TT organized by MA)**
TT 67.1–67.11	Thu	10:30–13:30	H4	**Oxides and Insulator Surfaces: Structure, Epitaxy and Growth (Joint session of O and TT organized by O)**
TT 68.1–68.9	Thu	10:30–13:00	H19	**Transport: Majorana Fermions**
TT 69.1–69.9	Thu	10:30–13:15	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport IV (Joint session of DS, HL, MA, MM, O and TT organized by O)**
TT 70.1–70.9	Thu	10:30–12:45	S053	**Graphene: Electronic Properties (Joint session of DS, DY, HL, MA, O and TT organized by O)**
TT 71.1–71.11	Thu	10:30–13:30	S054	**2D Materials beyond Graphene -Dynamics and Excitation (Joint session of DS, DY, HL, MA, O and TT organized by O)**
TT 72.1–72.8	Thu	14:45–17:15	H10	**Topological Insulators I (Joint session of DS, HL, MA, O and TT organized by HL)**
TT 73.1–73.10	Thu	15:00–18:00	H19	**Low-Dimensional Systems: Topological Order**
TT 74.1–74.5	Thu	15:00–17:45	H20	**Focus Session: Many-Body Interference and Quantum Statistical Physics (Joint session of DY and TT organized by DY)**
TT 75.1–75.4	Thu	15:00–16:00	H23	**Transport: Molecular Electronics and Photonics 2 (Joint session of CPP, DS, HL, MA, O and TT organized by TT)**
TT 76.1–76.13	Thu	15:00–18:15	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport V (Joint session of DS, HL, MA, MM, O and TT organized by O)**
TT 77.1–77.9	Thu	15:00–17:30	H34	**Multiferroics (Joint session of MA, DF, DS, KR and TT organized by MA)**
TT 78.1–78.63	Thu	15:00–18:30	Poster D	**Correlated Electrons: Poster Session**
TT 79.1–79.11	Thu	15:30–18:30	H21	**Superconductivity: Fe-based Superconductors - 122**
TT 80.1–80.9	Thu	16:00–18:30	H18	**Correlated Electrons: (General) Theory 2**
TT 81.1–81.7	Thu	16:15–18:30	H23	**Transport: Spintronics and Magnetotransport (Joint session of DS, HL, MA and TT organized by TT)**

TT 82.1–82.8	Thu	16:30–18:30	H22	**Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 2**
TT 83.1–83.5	Fri	9:30–12:15	H1	**Symposium on Frontiers of Electronic Structure Theory: Focus on Topology and Transport (SYES)** **(Joint symposium of DS, HL, MA, MM, O and TT organized by O)**
TT 84.1–84.8	Fri	9:30–12:00	H15	**Topological Insulators II** **(Joint session of DS, HL, MA, O and TT organized by O)**
TT 85.1–85.10	Fri	10:30–13:00	S051	**Graphene: Electronic Properties & Structure** **(Joint session of O and TT organized by O)**
TT 86.1–86.10	Fri	10:30–13:00	S051	**Graphene: Electronic Properties and Structure** **(Joint session of DS, DY, HL, MA, O and TT organized by O)**

Annual General Meeting of the Low Temperature Physics Division

Thursday 18:45 H19

TT 1: Tutorial: Correlations in Integrable Quantum Many-Body Systems

The tutorial is planned to present recent developments and ongoing activities in the theory of exact correlation functions of Heisenberg spin chains and their relatives, such as integrable bosonic and fermionic gases. Recent theoretical developments go beyond the calculation of just universal properties of many body systems as captured in Tomonaga-Luttinger liquid theory. By taking account of the full interactions of integrable Hamiltonians the complete correlations at large and short distances respectively small and large frequencies can be calculated. Due to substantial experimental advances integrable models of condensed matter physics can be realized for instance by ultra-cold quantum gases in traps.

Organizers: Hermann Boos and Andreas Klümper (Universität Wuppertal)

Time: Sunday 16:00–18:30 Location: H20

Tutorial TT 1.1 Sun 16:00 H20

Correlation functions of integrable models — •Frank Göhmann — Bergische Universität Wuppertal

This introductory tutorial reviews some of the progress in the theory of integrable quantum systems that led to the exact calculation of correlation functions of Heisenberg spin chains and related integrable quantum field theories. I shall mostly focus on two subjects: the factorization property of correlation functions of integrable models, discovered about 15 years ago, and the exact calculation and summation of matrix elements appearing in Lehmann representations of their correlation functions. Special emphasis will be put on methods which allow us to take into account the temperature dependence and on methods for calculating the long-time large-distance asymptotic behaviour of correlation functions.

Tutorial TT 1.2 Sun 16:45 H20

Non-Abelian anyons — •Holger Frahm — Institut für Theoretische Physik, Leibniz Universität Hannover

In this tutorial we shall discuss the construction and analysis of integrable many-body quantum systems built from non-Abelian anyons – objects with most exotic statistics under permutation whose states are protected against local perturbations by the existence of topological charges. They can appear as quasi-particle excitations in certain topological quantum liquids and are possibly realized in quantum Hall states at certain fractional filling factors or frustrated two-dimensional quantum magnets. Integrable models can provide unbiased insights into the nature of the collective states of many anyons formed in the presence of interactions.

We begin the tutorial with a brief review of the theoretical description of interacting many-anyon lattice models starting from the underlying fusion category. Within this framework a basis of operators for local interactions of anyons as well as the topological charges characterizing the many-anyon state are built. Finally, we show how by fine-tuning of the coupling constants the resulting models can be embedded into families of commuting operators and discuss strategies for the calculation of their spectral properties.

15 min. break

Tutorial TT 1.3 Sun 17:45 H20

Quantum quenches and equilibration of lattice and continuum systems — •Michael Brockmann — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

In this tutorial we will discuss the problem of relaxation and equilibration in closed quantum systems which are prepared in an off-equilibrium initial state. Quantum quenches are examples of such out of equilibrium situations. The focus will be on one-dimensional integrable theories where additional conservation laws heavily restrict the dynamics of the system.

I will briefly present two examples for which the steady state can be investigated by means of exact methods. The first example is a quench protocol where the ground state of a free many-particle bosonic theory unitarily evolves in time under the Lieb-Liniger Hamiltonian of δ-interacting repulsive bosons. In the second example the antiferromagnetic Néel state, the ground state of the spin-1/2 Ising chain, is released into the anisotropic Heisenberg spin chain. Using a variational method, the so-called quench action approach (QAA), one obtains the exact non-thermal steady state of the system in the thermodynamic limit, which correctly reproduces expectation values of local observables. Besides being rare cases of exact solutions of quench situations in truly interacting theories, those two quench protocols represent examples where a naive implementation of the generalized Gibbs ensemble (GGE) fails.

TT 2: Graphene: Theory (Joint session of DS, DY, HL, MA, O and TT organized by HL)

Time: Monday 9:30–12:30 Location: H17

TT 2.1 Mon 9:30 H17

Instantaneous Quantum Time Reversal Mirror in Graphene — •Phillipp Reck[1], Cosimo Gorini[1], Arseni Goussev[2], Mathias Fink[3], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Department of Mathematics and Information Sciences, Northumbria University, Newcastle Upon Tyne, UK — [3]Ecole Supérieure de Physique et Chimie Industrielle, CNRS, PSL Research University, Paris, France

The physicists' fascination for time inversion goes back a long time, as testified by the famous 19th-century argument between Loschmidt and Boltzmann concerning the arrow of time. Both metaphysical and practical considerations intrigued generations of scientists, who have ever since strived to devise and implement time-inversion protocols – in particular, different forms of "time mirrors" for classical waves such as sound- and electromagnetic-waves (see e.g. [1-2]), and recently an instantaneous time mirror for water waves [3].

Here we propose the realization of instantaneous Time Mirrors for quantum systems. These are controlled time discontinuities acting on wavefronts as mirrors in time and leading to distinct wavefunction echoes. More precisely, our Quantum Time Mirror exploits up to now unrelated concepts of wavefront time inversion and population reversal in two-level systems, the latter quintessential to spin echoes. It can be implemented in a relativistic Dirac-like system, e.g. graphene.

[1]M. Fink , IEEE Trans. Ultr. Ferroel. Freq. Control, 39, 555, (1992)

[2]G. Lerosey, et al., Phys. Rev. Lett. 92, 193904 (2004)

[3]V. Bacot, et al., preprint (2015)

TT 2.2 Mon 9:45 H17

Plasmon signature in Dirac-Weyl liquids — •Johannes Hofmann — TCM Group, Cavendish Laboratory, University of Cambridge, UK

I shall discuss theoretically as a function of temperature the plasmon mode arising in three-dimensional Dirac liquids, i.e., systems with linear chiral relativistic single-particle dispersion, within the random phase approximation. It is found that whereas no plasmon mode exists in the intrinsic (undoped) system at zero temperature, there is a well-defined finite-temperature plasmon with superlinear temperature dependence, rendering the plasmon dispersion widely tunable with temperature. The plasmon dispersion contains a logarithmic correction due to the ultraviolet-logarithmic renormalization of the electron

charge, manifesting a fundamental many-body interaction effect as in quantum electrodynamics. The plasmon dispersion of the extrinsic (doped) system displays a minimum at finite temperature before it crosses over to the superlinear intrinsic behavior at higher temperature, implying that the high-temperature plasmon is a universal feature of Dirac liquids irrespective of doping. This striking characteristic temperature dependence of intrinsic Dirac plasmons along with the logarithmic renormalization is a unique manifestation of the three-dimensional relativistic Dirac nature of quasiparticle excitations and serves as an experimentally observable signature of three-dimensional Dirac materials.

TT 2.3 Mon 10:00 H17

Finite temperature and electric field effects in the RKKY interaction in graphene and bilayer graphene — •Nicolas Klier[1], Sangeeta Sharma[2], Oleg Pankratov[1], and Sam Shallcross[1] — [1]Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7-B2, 91058 Erlangen — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction in Bernal stacked bilayer graphene [1,2] is shown to have a particularly rich dependence on temperature and a layer symmetry breaking electric field. Depending on whether we consider the chemical potential or particle number as the fixed variable we find that an electric field may tune the RKKY between ferromagnetic (FM) and anti-ferromagnetic (AFM) coupling, or an oscillatory and AFM coupling.

[1] N. Klier, S. Shallcross, and O. Pankratov, *P*hys. Rev. B **90**, 245118, 2014.
[2] N. Klier, S. Shallcross, S. Sharma, and O. Pankratov, *P*hys. Rev. B **92**, 205414, 2015.

TT 2.4 Mon 10:15 H17

The Electronic Structure of Graphene from Dyson-Schwinger Equations with Partially Screened Coulomb Interactions — •Manon Bischoff[1], Katja Kleeberg[2], Dominik Smith[2], Lorenz von Smekal[2], and Björn Wellegehausen[2] — [1]Johannes Gutenberg Universität, Mainz, Deutschland — [2]Justus Liebig Universität, Gießen, Deutschland

We have studied the possibility of a semimetal-insulator transition via spin-density or charge-density wave formation with partially screened Coulomb interactions in graphene from the coupled Dyson-Schwinger equations (DSEs) for the electronic excitations and their Lindhard screening on the honeycomb lattice. In the limit of purely static Lindhard screening these DSEs close on themselves and no further truncation is necessary. With appropriate boundary conditions they can then be solved numerically by fixed-point iteration. This is particularly efficient on graphical processing units (GPUs). After validating the static approximation from Monte-Carlo simulations on smaller lattices with appropriate boundary conditions, it allows to study much larger sheets than in the ab-initio simulations, e.g., to search for Miransky scaling, and to include cases where the latter break down because of a fermion-sign problem as for charge-density wave formation, for example.

TT 2.5 Mon 10:30 H17

Ab-initio lattice Monte-Carlo simulations of the Neck-disrupting Lifshitz transition in mono-layer graphene — •Michael Koerner, Dominik Smith, and Lorenz von Smekal — Institut fuer Theoretische Physik, Justus-Liebig-Universitaet Giessen

We study the effects of inter-electron interactions on the neck-disrupting Lifshitz transition, which is characterized by a change of topology of the Fermi surface. The Lifshitz transition is known to occur within a pure tight-binding description of mono-layer graphene when an external chemical potential drives the Fermi surface away from half-filling and across the saddles at the M-points. At these Van Hove singularities the density of states diverges logarithmically without interactions. We employ ab-intio Monte-Carlo simulations, which account for the full many-body physics of interacting electrons. We choose a partially screened Coulomb potential which combines the screening from localized electron states at short distances with the unscreened long-range Coulomb tails characteristic of graphene at half filling. Our goal is to determine whether interactions change the character of the topological transition, such that a real phase transition in the thermodynamic sense may occur, possibly in combination with chiral superconductivity.

TT 2.6 Mon 10:45 H17

Tight-binding description of spin-orbit coupling in graphene due to adatoms — •Susanne Irmer, Denis Kochan, Klaus Zollner, Martin Gmitra, Tobias Frank, and Jaroslav Fabian — University of Regensburg, Regensburg, Germany

We present realistic effective tight-binding models for proximity spin-orbit coupling in graphene due to adatoms at top, bridge, and hollow positions. The models are built from symmetry arguments and fitted to ab initio calculations for a variety of adsorbants, such as H [1], F [2], Cu, and CH3 [3]. For each of these adatoms we provide magnitudes for orbital couplings to the adsorbants, as well as the intrinsics, Rashba, and pseudospin-inversion asymmetry (PIA) couplings. Our models can be used to study spin relaxation, spin Hall effect, and spin transport using quantum transport models.

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] M. Gmitra, D. Kochan, J. Fabian, Phys. Rev. Lett. 110, 246602 (2013)
[2] S. Irmer, T. Frank, S. Putz, M. Gmitra, D. Kochan, J. Fabian, Phys. Rev. B 91, 115141 (2015)
[3] K. Zollner, T. Frank, S. Irmer, M. Gmitra, D. Kochan, J. Fabian, arXiv:1507.02820

30 min. Coffee Break

TT 2.7 Mon 11:30 H17

Ab initio studies of excitations in monolayer black phosphorus — •Tobias Frank[1], Marcin Kurpas[1], Martin Gmitra[1], Rene Derian[2], Ivan Stich[2], and Jaroslav Fabian[1] — [1]Universität Regensburg, Regensburg, Germany — [2]Slovak Academy of Sciences, Bratislava, Slovakia

Monolayer black phosphorus, or phosphorene, represents an ideal system to study many-body electron-electron and electron-hole interactions due to its strong anisotropy driven 1d electronic nature. In particular, the size of the fundamental band gap value and excitonic binding energies remain unresolved given the different gap values of 1.6 to 2.4 eV [1] obtained by many-body GW calculations. We present our contribution to this issue studying excitations in phosphorene employing quantum monte carlo (QMC) calculations. We show the evolution of finite size effects of the fundamental and optical gap, with respect to relatively large supercell sizes in the theoretical framework of diffusion monte carlo (DMC) explicitly including electronic correlations. Our studies point to a significant influence of electron correlation on the fundamental gap as well as to a strong anisotropic nature of the excitonic state. Furthermore we address the question of a multiconfigurational ground state in monolayer black phosphorus. 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] A. N. Rudenko, Shengjun Yuan, and M. I. Katsnelson, Phys. Rev. B 92 085419 (2015)

TT 2.8 Mon 11:45 H17

Phase structure of graphene from Hybrid Monte-Carlo simulations — •Pavel Buividovich[1], Lorenz von Smekal[2], Dominik Smith[2], and Maksim Ulybyshev[1] — [1]Regensburg University, Institute for Theoretical Physics, D-93053 Regensburg, Universitatstr. 31 — [2]Giessen University, Institute for Theoretical Physics, D-35392 Gießen, Heinrich-Buff-Ring 16

We study the phase structure of monolayer graphene in the parametric space of on-site and nearest-neighbour interactions using the Hybrid Monte-Carlo algorithm similar to those used in lattice QCD simulations. Our simulation code allows us to perform ab-initio simulations on lattices as big as 36x36 unit cells. We numerically determine the boundaries of the charge density wave, spin density wave and the Kekule distortion phases. We also confront the results with analytic studies based on Schwinger-Dyson equations, which allow to reach even larger lattice sizes, up to 5000x5000 unit cells.

TT 2.9 Mon 12:00 H17

Quantum Monte-Carlo study of graphene in external magnetic field — •Maksim Ulybyshev — Institute of Theoretical Physics, University of Regensburg, D-93053 Germany, Regensburg, Universitatsstrasse 31

Recent experimental results indicate that graphene turns into insulator in sufficiently strong magnetic field. However, the exact nature of this state is still elusive and there are some discrepancies between

theoretical predictions and experimental results. To resolve this discrepancies extensive simulations of graphene in external magnetic field were performed using Hybrid Monte Carlo algorithm. Insulating state was observed in agreement with experiment. Mass gap and various order parameters were measured.

TT 2.10 Mon 12:15 H17

Interaction-induced conductance from zero modes in a clean magnetic graphene waveguide — •Laura Cohnitz[1], Wolfgang Häusler[2,3], Alex Zazunov[1], and Reinhold Egger[1] — [1]Institut für Theoretische Physik, Heinrich-Heine-Universität, D-40225 Düsseldorf, Germany — [2]Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany — [3]Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany

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 at 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. We argue that this interaction-driven zero-mode conductor may also appear in other physical settings and is not captured by the conventional Tomonaga-Luttinger liquid description.

TT 3: Correlated Electrons: Frustrated Magnets - Pyrochlore Systems and Iridates

Time: Monday 9:30–13:00 Location: H20

TT 3.1 Mon 9:30 H20

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], Philipp Materne[1], Christopher 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) fluctuations upon cooling towards the NMR and neutron scattering spin frozen state 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 3.2 Mon 9:45 H20

Unusual spin frozen state in a frustrated pyrochlore system $NaCaCo_2F_7$ as observed by NMR — •R. Sarkar[1], J. W. Krizan[2], F. Brückner[1], R. J. Cava[2], and H.-H Klauss[1] — [1]IFP, TU Dresden, D-01069 Dresden, Germany — [2]Department of Chemistry, Princeton University, Princeton, NJ 08544, USA

We present ^{23}Na -and ^{19}F NMR results on the magnetically frustrated pyrochlore $NaCaCo_2F_7$ with a frustration index of $f = \theta_{CW}/T_f \sim 56$. Recent neutron scattering experiments proposed XY like antiferromagnetic spin clusters at low energies in $NaCaCo_2F_7$. ^{23}Na NMR -spectra reveal the presence of two magnetically non equivalent Na sites in conjunction with the local Co^{2+} spin structure. Below 3.6 K both the ^{23}Na -and ^{19}F spectra broaden due to the formation of static spin correlations. A huge reduction of the ^{19}F -and ^{23}Na NMR signal intensity hints at a quasi-static field distribution in $NaCaCo_2F_7$ in this regime. The ^{19}F spin-lattice relaxation rate $^{19}(1/T_1)$ exhibits a peak at around 2.9 K, at the same temperature range where ac and dc susceptibility data show a broad maximum. The character of the spin fluctuation appears to be isotropic. The overall temperature dependence of $^{19}(1/T_1)$ can be described by the BPP theory considering a fluctuating hyperfine field with an autocorrelation function. The correlation time of the autocorrelation function exhibits an activation behavior further indicating the spin-frozen state. While the present NMR studies suggest the spin frozen state at low temperatures, μSR investigations however reveal the presence of so called persistent spin dynamics down to 20 mK implying an exotic ground state in $NaCaCo_2F_7$.

TT 3.3 Mon 10:00 H20

Magnetoelastic properties of the quantum-spin-ice candidate $Yb_2Ti_2O_7$ — •T. Stöter[1,2,3], M. Doerr[1,2], S. Granovsky[1,2], Z.S. Wang[1,2,3], S. Erfanifam[3], E. Green[3], S. Zherlitsyn[1,3], J. Wosnitza[1,2,3], A. Maljuk[1,4], and S. Wurmehl[1,4] — [1]SFB 1143 — [2]TUD/IFP, Dresden — [3]HZDR, Dresden — [4]IFW, Dresden

Intriguing phenomena such as the occurrence of magnetic monopoles and a wide variety of ground states are associated to magnetic frustration. In a number of cases, elastic effects, e.g. lattice distortions, may result in the lifting of degeneracies or the appearance of new magnetic states. The rare-earth titanate $Yb_2Ti_2O_7$, where the magnetic Yb^{3+} ions form a pyrochlore spin network, is a prime example of a geometrically frustrated material, with numerous field-induced phases and strong ferromagnetic correlations below 170 mK. In order to characterize the magneto-elastic coupling in this material, we have investigated the thermal expansion, magnetostriction, and sound propagation in different dilution refrigerators between 60 mK and 1.5 K and large applied magnetic fields. At around 170 mK we find distinct anomalies in the expansion coefficient, acoustic properties, as well as the specific heat. Lattice anomalies in field hint to additional low temperature phases.

TT 3.4 Mon 10:15 H20

Suppression of Pauling's residual entropy in dilute spin ice $(Dy_{1-x}Y_x)_2Ti_2O_7$ — •S. Scharffe[1], O. Breunig[1], V. Cho[1], P. Laschitzky[1], M. Valldor[1,2], J. F. Welter[1], and T. Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

The spin ice $Dy_2Ti_2O_7$ is a geometrically frustrated spin system consisting of corner-sharing tetrahedra with an Ising anisotropy that aligns the spins along their local easy axes in the {111} direction. In the ground state configuration two spins point into and two out of each tetrahedron. The entropy of $Dy_2Ti_2O_7$ reveals a plateaulike feature close to Pauling's residual entropy around 0.5 K derived originally for water ice, but a distinct expansion towards lower temperature is prevented by ultraslow thermal equilibration. We present specific-heat data of $(Dy_{1-x}Y_x)_2Ti_2O_7$ and analyze the influence of nonmagnetic yttrium dilution on the low-temperature entropy. We find that these ultraslow thermal equilibration rapidly vanishes with increasing x, the low-temperature entropy systematically decreases, and its temperature dependence strongly increases[1]. From our data, a nondegenerate ground state can be derived for $(Dy_{1-x}Y_x)_2Ti_2O_7$ with intermediate dilution. This is in contrast to an expected zero-temperature residual entropy obtained from a generalization of Pauling's theory for dilute spin ice, but is supported by Monte Carlo simulations which are also compared to our results.

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

[1] Scharffe et al., PRB, **92**, 180405(R) (2015)

TT 3.5 Mon 10:30 H20

Determination of the spin Hamiltonian in the pyrochlore $Lu_2V_2O_7$ — •Kira Riedl[1], Harald O. Jeschke[1], Michel J.P. Gingras[2,3,4], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany — [2]Department of Physics and Astronomy, University of Waterloo, Ontario, N2L 3G1, Canada — [3]Perimeter Institute for Theoretical Physics, Waterloo, Ontario, N2L 2Y5, Canada

— [4]Canadian Institute for Advanced Research, 180 Dundas Street West, Suite 1400, Toronto, ON, M5G 1Z8, Canada

In the pyrochlore $Lu_2V_2O_7$ the vanadium ions form corner-sharing spin 1/2 tetrahedra. In order to find the corresponding spin Hamiltonian which captures the essential physics of the investigated compound we performed a tight-binding fit on the vanadium d orbitals using density functional theory. Since there is evidence that the Dzyaloshinskii-Moriya interaction (DMI) is important in this system, we considered spin-orbit coupling effects within our calculations.

A fitting procedure to the relativistic band structure enabled us to determine the strength of the spin-orbit coupling. In a second step, we calculated the energy parameters in the spin Hamitonian with the method of exact diagonalization and projection on low energy states. We were therefore able to evaluate the Heisenberg exchange, the DMI, and the symmetric tensor, only using *ab initio* information and reasonable values for the Hubbard interaction as well as for the Hund's coupling. Comparison with recent experimental results will be discussed.

15 min. break

TT 3.6 Mon 11:00 H20

Neutron scattering investigation of rare earth pyrochlore iridates and hafnates — •Erxi Feng[1], Yixi Su[1], Thomas Wolf[2], and Thomas Brueckel[3,1] — [1]Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, D-85747 Garching, Germany — [2]Institut für Festkörperphysik, Karlsruhe Institute of Technology KIT, D-76021 Karlsruhe, Germany — [3]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA- FIT, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Pyrochlore iridates and hafnates $A_2B_2O_7$ (A= rare earth ion, B=Ir, Hf), in which both the A-site and the B-site ions form corner-sharing tetrahedra, have recently attracted considerable research interests due to the presence of both strong spin-orbit coupling and geometrical frustration. $A_2B_2O_7$ displays an intriguing metal-to-insulator transition (MIT) driven by both thermodynamics and chemical pressure, which is suggested to coincide with possible magnetic order at the Ir^{4+} site. Moreover, the two sublattices of A^{3+} and Ir^{4+} might be magnetically coupled thus leading to novel magnetic behaviors. As a counterpart, $A_2B_2O_7$ compounds are insulator and the Hf4+ ion is nonmagnetic. Pyrochlore iridates and hafnates powders with light rare earth Pr and Nd were synthesized by standard solid state reaction. Combined X-ray and neutron powder diffraction refinements suggest that the samples are stoichiometric. In this presentation, our recent investigations of the magnetic ground states of these compounds via comprehensive neutron scattering techniques will be reported.

TT 3.7 Mon 11:15 H20

First-principles study of strong correlation effects in pyrochlore iridates — •Hiroshi Shinaoka[1], Shintaro Hoshino[2], Matthias Troyer[3], and Philipp Werner[4] — [1]Department of Physics, Saitama University, Japan — [2]Department of Basic Science, The University of Tokyo, Japan — [3]Theoretische Physik, ETH Zuerich, Switzerland — [4]Department of Physics, University of Fribourg, Switzerland

The pyrochlore iridates $A_2Ir_2O_7$ (A=Pr, Nd, Y, etc.) are an ideal system to study fascinating phenomena induced by strong electron correlations and spin-orbit coupling. In this talk, we study strong correlation effects in the prototype compound $Y_2Ir_2O_7$ using the local density approximation and dynamical mean-field theory (LDA+DMFT) [1]. We map out the phase diagram in the space of temperature, on-site Coulomb repulsion U, and filling. Consistent with experiments, we find that an all-in/all-out ordered insulating phase is stable for realistic values of U. We reveal the importance of the hybridization between $j_{eff} = 1/2$ and $j_{eff} = 3/2$ states under the Coulomb interaction and trigonal crystal field. We demonstrate a substantial band narrowing in the paramagnetic metallic phase and non-Fermi liquid behavior in the electron/hole doped system originating from long-lived quasi-spin moments induced by nearly flat bands. We further compare our results with recent experimental results of $Eu_2Ir_2O_7$ under hydrostatic pressure [2].

[1] H. Shinaoka, S. Hoshino, M. Troyer, P. Werner, PRL **115**, 156401 (2015)
[2] G. Prando, R. Dally, W. Schottenhamel, Z. Guguchia, S.-H. Baek, R. Aeschlimann, A. U. B. Wolter, S. D. Wilson, B. Büchner, M. J. Graf, arXiv:1511.03037

TT 3.8 Mon 11:30 H20

Metal-insulator transition of pyrochlore iridates and their topological properties — •Hongbin Zhang[1,2], Kristjan Haule[2], and David Vanderbilt[2] — [1]Materialwissenschaft, TU Darmstadt Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany — [2]Department of Physics and Astronomy, Rutgers University, 136 Frelinghuysen Road, NJ-08854, USA

The interplay of spin-orbit coupling and electronic correlations can lead to many fascinating physical properties, where iridates are a promising playground. Combining density functional theory (DFT) and embedded dynamical mean-field theory (DMFT) methods, we study the metal-insulator transition in $R_2Ir_2O_7$ (R=Y, Eu, Sm, Nd, Pr, and Bi) and the topological nature of the insulating compounds. Accurate free energies evaluated using the charge self-consistent DFT+DMFT method reveal that the metal-insulator transition occurs for an A-cation radius between that of Nd and Pr, in agreement with experiments. The all-in-all-out magnetic phase, which is stable in the Nd compound but not the Pr one, gives rise to a small Ir^{4+} magnetic moment of $\approx 0.5\mu_B$ and opens a sizable correlated gap. We demonstrate that within this state-of-the-art theoretical method, the insulating bulk pyrochlore iridates are topologically trivial.

TT 3.9 Mon 11:45 H20

Specific heat study of the iridium double perovskite Sr_2YIrO_6 — •Laura T. Corredor, Kaustuv Manna, Gizem Aslan Cansever, Sebastian Gass, Andreas Zimmermann, Tushar Dey, Christian Blum, Andrey Maljuk, Sabine Wurmehl, Anja Wolter, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research IFW, Institute for Solid State Research, 01069 Dresden, Germany

Recently, Mott insulators with a d^4 electronic configuration were predicted to show superexchange-driven quantum phase transitions. Double perovskites $R_2MM'O_6$ with M'^{3+} ion, yielding a formal oxidation state of Ir^{5+} with $5d^4$ electronic configuration, may be candidates to verify or discard such transitions and its impact on the magnetic structure. According to the strong spin-orbit coupling J_{eff} model, a non-magnetic ground state is expected. Such material is realized in Sr_2YIrO_6. Nevertheless, it is claimed [1] that a strong non-cubic crystal field together with a "intermediate-strength" spin-orbit coupling, would lead to a different ground state configuration and to antiferromagnetic behavior with $T_N = 1.3$ K. Also, anomalies in the specific heat were associated to this novel magnetism. In this work, we present magnetic and thermodynamic characterization of Sr_2YIrO_6 single crystals. No long magnetic order was found. The magnetic contribution to the specific heat was calculated, finding a Schottky anomaly due to magnetic impurities. Further analysis suggests non-negligible spin correlations, which nonetheless, are not associated with long range magnetic ordering.

[1] G.Cao et al., PRL **112**, 056402 (2014).

TT 3.10 Mon 12:00 H20

On the search for magnetic correlations in double perovskites — •Franziska Hammerath[1,2], Rajib Sarkar[1], Sirko Kamusella[1], C. Baines[3], H.-H. Klauss[1], T. Dey[2], Gizem Aslan Cansever[2], Kaustuv Manna[2], Andreas Zimmermann[2], Andrey Maljuk[2], Mihai Sturza[2], Dmitriy Efremov[2], Sabine Wurmehl[2], and Bernd Büchner[2] — [1]Institute for Solid State Physics, Dresden Technical University, TU Dresden, 01062 Dresden, Germany — [2]IFW Dresden, Institute for Solid State Research, PF 270116, 01171 Dresden, Germany — [3]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen, PSI, Switzerland

The cubic double perovskite Ba_2YIrO_6 has been investigated by the local probe techniques NMR and μSR. Both methods confirm the absence of long range order in this compound, but observe signatures of magnetic correlations: The NMR spin-lattice relaxation rate suggests the presence of growing magnetic correlations at low temperatures. An increase of the μSR spin-lattice relaxation rate confirms the presence of weak magnetism. These findings cannot be explained by the recently suggested excitonic type of magnetism [1], but also go beyond a simple nonmagnetic ground state picture of the $5d^4$ ($J_{eff} = 0$) electronic configuration of Ir^{5+}. In the monoclinic analog Sr_2YIrO_6, the NMR line width and spin-lattice relaxation rates reveal a nonmagnetic behavior, in contrast to a first report [2], but in line with a recent study [3].

[1] G. Khaliullin, PRL **111**, 197201 (2013).
[2] G. Cao *et al.*, PRL **112**, 056402 (2014).

[3] B. Ranjbar *et al.*, Inorg. Chem. **54**, 10468 (2015).

TT 3.11 Mon 12:15 H20

High-field multi-frequency ESR spectroscopy of La_2CuIrO_6 — •Stephan Fuchs[1], Vladislav Kataev[1], Kaustuv Manna[1], Sabine Wurmehl[1], Anup Kumar Bera[3], Andrey Malyuk[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 — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

We will present the electron spin resonance results of the double perovskite La_2CuIrO_6. This material provides a playground to examine the magnetic interactions in a 5d transition metal oxide with strong spin-orbit coupling. Measurements of the static magnetization M(T,H) show an antiferromagnetic ordering at $T_{AFM} = 74$ K and a weak ferromagnetic moment below 54 K. ESR measurements of the powder sample were carried out for several temperatures and frequencies to determine the g-factor and the magnetic exaction gap. Our goal is to identify the origin of the ferromagnetic contribution with ESR. We observe an opening of the ferromagnetic gap at T=93 K ($> T_{AFM}$) which continuously develops over the T_{AFM} down to low temperature. The complex interaction of the Cu- and Ir-spin gives rise to the continuous shift of the g-factor: By decreasing the temperature, the Ir spins are getting progressively more involved in the resonance of the statically ordered Cu spin lattice due to exchange coupling between the two sublattices. We conclude that the weak ferromagnetic component in La_2CuIrO_6 is intrinsic which points at a noncollinear spin-structure in the ordered state.

TT 3.12 Mon 12:30 H20

Single crystal growth of α-Li_2IrO_3 from separated educts — •Friedrich Freund, Anton Jesche, Ina-Marie Pietsch, and Philipp Gegenwart — EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany

Hexagonal iridates like α-Li_2IrO_3 are promising candidates for the realization of the Kitaev exchange interaction, which describes an anisotropic and bonding dependent interaction that can lead to novel types of spin liquid behavior. We report a method to grow for the first time single crystals of α-Li_2IrO_3. This method is using separated educts and could also be used to grow single crystals of other honeycomb transition metal oxides such as Li_2RuO_3. Besides the discussion of the new crystal growth method, we will present the structural and magnetic properties.

TT 3.13 Mon 12:45 H20

Neutron scattering signatures of the 3D hyper-honeycomb Kitaev quantum spin-liquid — •Adam Smith[1], Johannes Knolle[1], Dmitry L. Kovrizhin[1,2], John T. Chalker[3], and Roderich Moessner[4] — [1]T.C.M. Group, Cavendish Laboratory, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — [2]RRC Kurchatov Institute, 1 Kurchatov Square, Moscow 123182, Russia — [3]Theoretical Physics, Oxford University, 1 Keble Road, Oxford OX1 3NP, United Kingdom — [4]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany

Motivated by recent synthesis of the hyper-honeycomb material β-Li_2IrO_3, we study the dynamical structure factor (DSF) of the corresponding 3D Kitaev quantum spin-liquid (QSL), whose fractionalised degrees of freedom are Majorana fermions and emergent flux-loops. Properties of this 3D model are known to differ in important ways from those of its 2D counterpart - it has finite-temperature phase transition, as well as distinct features in Raman response. We show, however, that the qualitative behaviour of the DSF is broadly dimension-independent. Characteristics of the 3D DSF include a response gap even in the gapless QSL phase and an energy dependence deriving from the Majorana fermion density of states. Since the majority of the response is from states containing a single Majorana excitation, our results suggest inelastic neutron scattering as the spectroscopy of choice to illuminate the physics of Majorana fermions in Kitaev QSLs.

TT 4: Dynamics in many-body systems: Equilibriation and localization (Joint session of DY and TT organized by DY)

Time: Monday 9:30–12:45 Location: H47

TT 4.1 Mon 9:30 H47

Dynamical thermalization in Bose-Hubbard systems — •Peter Schlagheck[1] and Dima L. Shepelyansky[2] — [1]Département de Physique, Université de Liège, Belgium — [2]Laboratoire de Physique Théorique du CNRS, IRSAMC, Université de Toulouse UPS, France

A bosonic many-body system can exhibit the Bose-Einstein distribution in its single-particle eigenstates not only if it is coupled to a heat and particle reservoir, but also if it is subject to a two-body interaction of moderately low strength which couples the single-particle eigenstates with each other. We numerically verify this dynamical thermalization conjecture within disordered Bose-Hubbard rings of finite size whose parameters are chosen such that the dynamics of the system can be expected to be ergodic [1]. This allows one to associate with each many-body eigenstate of the Bose-Hubbard system well-defined (positive or negative) values for the effective temperature and the effective chemical potential which depend on the energy per particle of the eigenstate under consideration [1]. With this information one can then predict the populations of single-particle eigenmodes within each many-body eigenstate of the system according to the Bose-Einstein distribution, without knowing more details about the quantum dynamics of the many-body system.

[1] P. Schlagheck and D. L. Shepelyansky, arXiv:1510.01864.

TT 4.2 Mon 9:45 H47

Stationary state after a quench to the Lieb-Liniger from rotating BECs — •Leda Bucciantini — Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

We study long-time dynamics of a bosonic system after suddenly switching on repulsive delta-like interactions. As initial states, we consider two experimentally relevant configurations: a rotating BEC and two counter-propagating BECs with opposite momentum, both on a ring. In the first case, the rapidity distribution function for the stationary state is derived analytically and it is given by the distribution obtained for the same quench starting from a BEC, shifted by the momentum of each boson. In the second case, the rapidity distribution function is obtained numerically for generic values of repulsive interaction and initial momentum. The significant differences for the case of large versus small quenches are discussed.

TT 4.3 Mon 10:00 H47

Short time propagation in interacting bosonic systems — •Benjamin Geiger, Quirin Hummel, Juan-Diego Urbina, and Klaus Richter — Institut für Theoretische Physik Universität Regensburg, 93040 Regensburg, Germany

We present a formalism to calculate thermodynamic properties of interacting bosonic gases as well as the smooth (Weyl) contribution to density of states by means of short-time propagation, and compare its analytical predictions against quantum integrable models. As an essential input of our approach, we were able to construct the many-body propagator for a one-dimensional unconfined bosonic gas with delta interactions of variable strength. Using this propagator we can give short-time approximations for the Lieb-Liniger model and non-integrable systems including external harmonic potentials. Furthermore we can think of using the spatial information and the time dependence of the propagator to calculate e.g. two-point correlations or to investigate quantum quenches.

TT 4.4 Mon 10:15 H47

Equilibration in many-body localised systems — Mathis Friesdorf, Albert Werner, •Marcel Goihl, Winton Brown, and Jens Eisert — Freie Universität Berlin

The effect of many-body localisation (MBL) is connected to an intriguing class of systems that fail to thermalise. Due to the randomness present in these models, both particles and energies remain largely confined to local regions. This prevents the relaxation of excitations and thus leads to a local memory of the precise initial conditions even after long evolution times. Based on a phenomenological model of

MBL, we examine the time evolution of these systems and explore the role of local constants of motion, which are intrinsically present if energy is localised. We show that despite the fact that particles and energy are localised, information is able to propagate over arbitrary distances. Following this information theoretical viewpoint, we capture equilibration in MBL systems and derive time scales thereof. We connect our findings to signatures measurable in optical lattice architectures, thus allowing for the distinction of Anderson localisation and true MBL based solely on existing measurement techniques.

TT 4.5 Mon 10:30 H47

The eigenstate thermalization hypothesis as driving force behind initial state independent equilibration in closed quantum systems — •Christian Bartsch and Jochen Gemmer — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, D-49069 Osnabrück

We analyze the long time behavior of non-equilibrium expectation value dynamics for finite closed quantum systems considering very general Hamiltonians and observables. For a certain class of generic, i.e., experimentally realistic, initial states we analytically find that the long time expectation value depends on the concrete initial state and in general deviates from the expected average equilibrium value unless the eigenstate thermalization hypothesis (ETH) is fulfilled. We call this behavior stick effect. The initial states may be prepared by exposition of the system to a super bath in combination with an additional potential which depends on the regarded observable, thus the system is explicitly out of equilibrium and the initial state is correlated with both the Hamiltonian and the observable, i.e., the situation is not covered by established investigations involving typicality in terms of the Haar measure. The results suggest that the ETH may serve not only as a sufficient but also as a necessary condition for initial state independent equilibration. Numerics for a specific class of integrable quantum magnets, which does not fulfill the ETH, illustrate the findings.

TT 4.6 Mon 10:45 H47

Fluctuations, meta-stability and symmetry-breaking in open many-body systems — •Henrik Wilming[1], Albert H. Werner[1], Jens Eisert[1], and Michael J. Kastoryano[2] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany — [2]NBIA, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, DK

It is known that finite fluctuations of densities in thermal states correspond to the existence of several phases. In the case of fluctuations in order-parameters, they lead to the existence of spontaneous symmetry-breaking. Such results are purely kinematic in that they do not show how these states are prepared by nature.

Here, we consider the corresponding dynamical question: We assume that a state with finite fluctuations in a density is prepared by a dissipative Markovian short-range dynamics that is in detailed balance and show that such dynamics necessarily also has different meta-stable states, which converge to steady-states on (quasi-)local observables in the thermodynamic limit. In the case of fluctuating order-parameters we show the existence of explicitly symmetry-breaking meta-stable states and construct dissipative Goldstone-modes on top of them.

The existence of such meta-stable states shows that it is inherently difficult to prepare a many-body state with strong long-range correlations by short-range dissipative processes fulfilling detailed balance. Our results hold on regular lattices in arbitrary spatial dimensions and are constructive in the sense that we explicitly write down the meta-stable states.

15 min. break

TT 4.7 Mon 11:15 H47

Approaching equilibrium: Fermionic Gaussification — •Marek Gluza[1], Christian Krumnow[1], Mathis Friesdorf[1], Christian Gogolin[2,3], and Jens Eisert[1] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Berlin, Germany — [2]ICFO-The Institute of Photonic Sciences, Mediterranean Technology Park, Barcelona, Spain — [3]Max-Planck-Institut für Quantenoptik, Garching, Germany

When and by which mechanism do closed quantum many-body systems equilibrate? This fundamental question lies at the very basis of the connection between thermodynamics, many-body quantum mechanics and condensed matter theory. In the setting of free fermionic evolutions, we rigorously capture the time evolution in abstract terms and uncover the underlying mechanism how local memory of the initial conditions is forgotten. Specifically, starting from an initially short range correlated fermionic states which can be very far from Gaussian, we show that if the Hamiltonian provides sufficient transport, the system approaches a state that locally cannot be distinguished from a corresponding Gaussian state. In this way, strongly correlated states, as encountered in the Fermi-Hubbard model, will become locally Gaussian during the evolution under a hopping Hamiltonian, leading to density-density correlations that factor according to Wick's theorem. For experimentally relevant instances of ultra-cold fermions in optical lattices, our result implies equilibration on realistic physical time scales. Moreover, we characterise the equilibrium state, finding an instance of a rigorous convergence to a Generalized Gibbs ensemble.

TT 4.8 Mon 11:30 H47

Controlling Fluctuations in Parametrically Driven Oscillators and Lattices — •Beilei Zhu and Ludwig Mathey — ZOQ/ILP, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

We consider an oscillator parametrically and periodically driven at a high frequency . In the quantum limit we obtain an effective Hamiltonian in the interaction picture analytically via Magnus Expansion. We compare this analytical result with a numerical one, which is developed in the classic limit in the Langevin formalism. The simulation results show that the fluctuations of the oscillator coordinates are reduced at high driving frequencies and moderate driving amplitudes. We also obtain qualitatively similar results in a lattice of parametric oscillators.

TT 4.9 Mon 11:45 H47

Equilibration of isolated quantum systems due to restrictions in the experimental set-up — •Ben Niklas Balz — Bielefeld University, Germany

We will explore in what sense and under which conditions isolated quantum many-body systems equilibrate. To estimate the deviations from the equilibrium state a more realistic distinguishability measure than the ones used in [1,2] will be developed, taking into account how often observables with a certain set of outcomes are measured. As a consequence new insights which physical parameters influence equilibration dynamics in what way can be gained. This might be of theoretical importance contributing to the understanding of thermalization [3] or can be used to give more accurate bounds on equilibration times [4,5].

[1]Peter Reimann. Physica Scripta, 86(5), 2012.
[2]Anthony J Short. New Journal of Physics, 13(5):053009, 2011.
[3]Peter Reimann. New Journal of Physics, 17(5):055025, 2015.
[4]D. Hetterich, M. Fuchs, and B. Trauzettel. ArXiv, June 2015.
[5]L. P. Garcia-Pintos, N. Linden, A. S. L. Malabarba, A. J. Short, and A. Winter. ArXiv e-prints, September 2015.

TT 4.10 Mon 12:00 H47

Reduced fluctuations in dissipative parametric oscillators — •Tobias Rexin, Beilei Zhu, and Ludwig Mathey — Zentrum für Optische Quantentechnologien und Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany

In this work we describe the non-equilibrium effects of a dissipative parametric oscillator system for which we derive an effective time-independent Hamiltonian via Magnus Expansion. The analytical result shows reduced variance in the high driving frequency and moderate driving amplitude regime, which also coincides with numerical results from the Langevin Equations. A chain of parametric oscillators exhibits similiar behavior.

TT 4.11 Mon 12:15 H47

Time evolution of the electron distribution function of thin copper films probed with broadband femtosecond optical pulses — •Manuel Obergfell and Jure Demsar — Universität Mainz

The time-resolved dynamics of the optical constants of thin copper films has been measured in the visible range. The photoinduced changes in reflectivity and transmission are based on the changes to the electron distribution function at the Fermi level. The dielectric function of copper is modelled at the d-band to Fermi level transition at photon energies up to 3 eV. With a low amount of sample dependent parameters the matching to the temperature dependence of the dielectric function of copper is achieved. Therefore we can reproduce stan-

dard thermomodulation. To extract the electron distribution function time dependently, the deconvolution is performed by matrix inversion. Our results demonstrate a highly non-thermal electronic distribution up to time delays of more than 1 ps depending on excitation density, at odds with the Two-Temperature model assumption. We extract the electron-phonon coupling constant from these data and compare the results to several recent theoretical models.

TT 4.12 Mon 12:30 H47

Adsorption-desorption kinetics of soft particles onto surfaces — •Brendan Osberg and Ulrich Gerland — Complex Biosystems, Physik-Department, Technische Universitaet Muenchen, Garching, Germany

A broad range of physical, chemical, and biological systems feature processes in which particles randomly adsorb on an extended substrate. Theoretical models usually assume hard (mutually impenetrable) particles, but in soft matter physics the adsorbing particles can be effectively compressible, implying soft interaction potentials. We recently studied the kinetics of such soft particles adsorbing onto one-dimensional substrates, identifying three novel phenomena: (i)gradual density increases, or 'cramming', replaces the usual jamming behavior seen in hard particles, (ii) a density overshoot can occur (only for soft particles) on a time scale set by the desorption rate, and (iii) relaxation rates of soft particles increase with particle size (on a lattice), while hard particles show the opposite trend. The latter occurs since unjamming requires desorption and many-bodied reorganization to equilibrate -a process that is generally very slow. Here we extend this analysis to a two-dimensional substrate, focusing on the question of whether the adsorption-desorption dynamics of particles in two dimensions are similarly enriched by the introduction of soft interactions. Application to experiments, for example the adsorption of fibrinogen on two-dimensional surfaces, will be discussed.

TT 5: Transport: Quantum Coherence and Quantum Information Systems - Experiment (Joint session of HL, MA and TT organized by TT)

Time: Monday 9:45–13:00 Location: H22

TT 5.1 Mon 9:45 H22

Tunable coupling between fixed-frequency superconducting transmon qubits — •Stefan Filipp[1], David C. McKay[2], Easwar Magesan[2], Antonio Mezzacapo[2], Jerry M. Chow[2], and Jay M. Gambetta[2] — [1]IBM Research - Zurich, 8803 Rueschlikon, Switzerland — [2]IBM TJ Watson Research Center, Yorktown Heights, NY, USA

The controlled realization of qubit-qubit interactions is essential for both the physical implementation of quantum error-correction codes and for reliable quantum simulations. Ideally, the fidelity and speed of corresponding two-qubit gate operations is comparable to those of single qubit operations. In particular, in a scalable superconducting qubit architecture coherence must not be compromised by the presence of additional coupling elements mediating the interaction between qubits. Here we present a coupling method between fixed-frequency transmon qubits based on the frequency modulation of an auxiliary circuit coupling to the individual transmons. Since the coupler remains in its ground state at all times, its coherence does not significantly influence the fidelity of consequent entangling operations. Moreover, with the possibility to create interactions along different directions, our method is suited to engineer Hamiltonians with adjustable coupling terms. This property can be utilized for quantum simulations of spins or fermions in transmon arrays, in which pairwise couplings between adjacent qubits can be activated on demand.

TT 5.2 Mon 10:00 H22

Concentric transmon qubit featuring fast tunability and an anisotropic magnetic dipole moment — •Jochen Braumüller[1], Martin Sandberg[2], Michael R. Vissers[2], Andre Schneider[1], Steffen Schlör[1], Lukas Grünhaupt[1], Hannes Rotzinger[1], Michael Marthaler[1], Alexander Lukashenko[1], Amadeus Dieter[1], Alexey V. Ustinov[1,3], Martin Weides[1,4], and David P. Pappas[2] — [1]Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]National Institute of Standards and Technology, Boulder, Colorado 80305, USA — [3]National University of Science and Technology MISIS, Moscow 119049, Russia — [4]Johannes Gutenberg University, Mainz, 55128 Mainz, Germany

We present a planar qubit design based on a superconducting circuit that we call concentric transmon. While employing a straightforward fabrication process using Al evaporation and lift-off lithography, we observe qubit lifetimes and coherence times in the order of $10\,\mu$s. We systematically characterize loss channels such as incoherent dielectric loss, Purcell decay and radiative losses. The implementation of a gradiometric SQUID loop allows for a fast tuning of the qubit transition frequency and therefore for full tomographic control of the quantum circuit. Due to the large loop size, the presented qubit architecture features a strongly increased magnetic dipole moment as compared to conventional transmon designs. This renders the concentric transmon a promising candidate to establish a site-selective passive direct $\hat{Z}$ coupling between neighboring qubits, being a pending quest in the field of quantum simulation.

TT 5.3 Mon 10:15 H22

Quasiparticle-Induced Decoherence of Microscopic Two-Level-Systems in Superconducting Qubits — •Alexander Bilmes[1], Jürgen Lisenfeld[1], Sebastian Zanker[1], Michael Marthaler[2], Gerd Schön[2], Georg Weiss[1], and Alexey V. Ustinov[1] — [1]PHI, KIT, 76131 Karlsruhe, Germany — [2]TFP, KIT, 76131 Karlsruhe, Germany

Parasitic Two-Level-Systems (TLS) are one of the main sources of decoherence in superconducting nano-scale devices such as SQUIDs, resonators and quantum bits (qubits), although the TLS' microscopic nature remains unclear. We use a superconducting phase qubit to detect TLS contained within the tunnel barrier of the qubit's Al/AlOx/Al Josephson junction. If the TLS transition frequency lies within the $6-10\,$GHz range, we can coherently drive it by resonant microwave pulses and access its quantum state by utilizing the strong coupling to the qubit. Our previous measurements of TLS coherence in dependence of the temperature indicate that quasiparticles (QPs), which diffuse from the superconducting Al electrodes into the oxide layer, may give rise to TLS energy loss and dephasing [1]. Here, we probe the TLS-QP interaction using a reliable method of *in-situ* QP injection via an on-chip dc-SQUID that is pulse-biased beyond its switching current. The QP density is calibrated by measuring associated characteristic changes to the qubit's energy relaxation rate. We will present experimental data which show the QP-induced TLS decoherence in good agreement to theoretical predictions.

[1] J. Lisenfeld et al., PRL **105**, 230504 (2010)

TT 5.4 Mon 10:30 H22

Transmon qubits enter circuit nano-electromechanics — •Daniel Schwienbacher[1,2], Matthias Pernpeintner[1,2,3], Friedrich Wulschner[1,2], Philip Schmidt[1,2,3], Frank Deppe[1,2,3], Achim Marx[1], Rudolf Gross[1,2,3], and Hans Huebl[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

The field of cavity nano-electromechanics combines nano-scale mechanical elements with microwave circuits for the investigation of the light-matter interaction on a quantum level. In this context ground state cooling, electromechanically induced transparency effects, as wells as state transfer between the mechanical and photonic modes have been demonstrated. Recently, Abdi et al.[1] have proposed the integration of a nanomechanical beam into the capacitor of a transmon qubit, which is in turn coupled to a microwave resonator and predicted enhanced electro-mechanical coupling rates as well as the preparation of mechanical Fock states and the generation of three-partite entanglement. Here, we present an experimental study concerning the integration of a nanomechanical beam, a transmon qubit, and a microwave resonator on a single chip. We will discuss fabricational aspects and first spectroscopy data of the device.

We thankfully acknowledge financial support by the DFG via the collaborative research center SFB 631.

[1] Mehdi Abdi et al., PRL **114**, 173602 (2015)

TT 5.5 Mon 10:45 H22

Thermal microwave states acting on a superconducting qubit — •Jan Goetz[1,2], Miriam Müting[1,2], Max Haeberlein[1,2], Friedrich Wulschner[1,2], Edwar Xie[1,2,3], Peter Eder[1,2,3], Michael Fischer[1,2], Frank Deppe[1,2], Kirill Fedorov[1,2], Hans Hübl[1,2], Frank Deppe[1,2,3], Achim Marx[1], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 München, Germany

We analyze the influence of broadband thermal states in the microwave regime on the coherence properties of a superconducting (transmon) qubit coupled to a transmission line resonator. We generate the thermal states inside the resonator by heating a 30 dB attenuator to emit blackbody radiation into a transmission line. In the absence of thermal fluctuations, the qubit coherence time is limited by relaxation. We find that the relaxation rate is almost unaffected by the presence of a thermal field inside the resonator. However, such states induce significant dephasing which increases quadratically with the number of thermal photons, whereas for a coherent population of the resonator, the increase shows a linear behavior. These results confirm the different photon statistics, being Poissonian for a coherent population and super-Poissonian for a thermal population of the resonator.

This work is supported by the German Research Foundation through SFB 631 and FE 1564/1-1, EU projects CCQED, PROMISCE, the doctorate program ExQM of the Elite Network of Bavaria.

TT 5.6 Mon 11:00 H22

Displacement of squeezed propagating microwave states — •Kirill G. Fedorov[1], P. Yard[1,2], S. Pogorzalek[1,2], P. Eder[1,2,3], M. Fischer[1,2,3], J. Goetz[1,2], F. Wulschner[1,2], E. Xie[1,2,3], 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, Technische Universität München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 München, Germany

The displacement of propagating quantum states of light is a fundamental operation for quantum communication. It can be applied to fundamental studies of macroscopic quantum coherence and has an important role in quantum teleportation protocols with continuous variables. We study an experimental implementation of this operation for propagating squeezed microwave states. We generate these states using a Josephson parametric amplifier and implement the displacement operation using a specific cryogenic directional coupler. We demonstrate that even for strong displacement amplitudes we do not observe any degradation of the reconstructed quantum states. Furthermore, we confirm that path entanglement generated using displaced squeezed states, also stays constant over a wide range of the displacement power.

We acknowledge support by the German Research Foundation through SFB 631 and FE 1564/1-1, the EU project PROMISCE, and Elite Network of Bavaria through the program ExQM.

15 min. break

Invited Talk TT 5.7 Mon 11:30 H22

Coherent Suppression of Quasiparticle Dissipation in a Superconducting Artificial Atom — •Ioan Pop — Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — Department of Applied Physics, Yale University, New Haven, CT 06520, USA

We demonstrate immunity to quasiparticle dissipation in a Josephson junction. At the foundation of this protection rests a prediction by Brian Josephson from fifty years ago: the particle-hole interference of superconducting quasiparticles when tunneling across a Josephson junction [1]. The junction under study is the central element of a fluxonium artificial atom, which we place in an extremely low loss environment and measure using radio-frequency dispersive techniques [2]. Furthermore, by using a quantum limited amplifier (a Josephson Parametric Converter) we can observe quantum jumps between the 0 and 1 states of the qubit in thermal equilibrium with the environment. The distribution of the times in-between the quantum jumps reveals quantitative information about the population and dynamics of quasiparticles[3]. The data is entirely consistent with the hypothesis that our system is sensitive to single quasiparticle excitations, which opens new perspectives for quasiparticle monitoring in low temperature devices.

[1] B. D. Josephson, Physics Letters **1**, 251 (1962)
[2] I. M. Pop et al., Nature **508** (2014)
[3] U. Vool et al., PRL **113** (2014)

TT 5.8 Mon 12:00 H22

Tunable superconducting resonators with integrated trap structures for coupling with ultracold atomic gases — •Benedikt Ferdinand[1], Daniel Bothner[1,2], Dominik Wiedmaier[1], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany — [2]Kavli Institute of Nanoscience, Delft University of Technology, PO Box 5046, 2600 GA, Delft, The Netherlands

We intend to investigate a hybrid quantum system where ultracold atomic gases play the role of a long-living quantum memory, coupled to a superconducting qubit via a coplanar waveguide transmission line resonator. As a first step we developed a resonator chip containing a Z-shaped trapping wire for the atom trap. In order to suppress parasitic resonances due to stray capacitances, and to achieve good ground connection we use hybrid superconductor - normal conductor chips. As an additional degree of freedom we add a ferroelectric capacitor making the resonators voltage-tunable. We furthermore show theoretical results on the expected coupling strength between resonator and atomic cloud.

TT 5.9 Mon 12:15 H22

Quantum correlations in microwave frequency combs — •Thomas Weissl[1], Erik Tholén[2], Daniel Forchheimer[1,2], and David B. Haviland[1] — [1]KTH- Royal Institute of Technology, 106 91 Stockholm, Sweden — [2]Intermodulation Products AB, 823 93 Segersta, Sweden

Non-linear superconducting resonators are used as parametric amplifiers in circuit quantum electrodynamics experiments [1]. When pumped below threshold the pump correlates vacuum fluctuations in the signal and idler bands giving rise to two-mode squeezed vacuum. When a non-linear oscillator is pumped with a frequency comb complex multipartite entangled states can be created as demonstrated in similar experiments in the optical domain [2]. We present a method to generate and measure microwave frequency combs by up- and down-conversion from intermediate frequencies. The comb is generated and analyzed using a multi-frequency lock-in amplifier. From transmission measurements we extract correlation- and quasi-probability functions.

[1] E. Tholén et al., APL **90**, 253509 (2007)
[2] M. Chen et al., PRL **112**, 120505 (2014)

TT 5.10 Mon 12:30 H22

Microwave experiments with quantum phase-slip in superconducting AlO_x nanowires — •Sebastian T. Skacel[1], Marco Pfirrmann[1], Jan N. Voss[1], Micha Wildermuth[1], Julian Münzberg[1], Lucas Radtke[1], Sebastian Probst[1], Martin Weides[1,2], J. E. Mooij[1,3], Hannes Rotzinger[1], and Alexey V. Ustinov[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, D-76131 Karlsruhe, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, D-55128 Mainz, Germany — [3]Kavli Institute of Nanoscience, Delft University of Technology, 2628 CJ Delft, The Netherlands

Superconducting nanowires in the quantum phase slip (QPS) regime allow to study the flux and phase dynamics in duality to Josephson junction systems. We experimentally study QPS effects of nanowires which are embedded in a resonant microwave circuit. The samples are probed at ultra-low microwave power and applied magnetic field at mK temperatures. The AlO_x nanowires, with a sheet resistance in the kΩ range, are fabricated by sputter deposition of aluminium in a controlled oxygen atmosphere. The wires are defined with conventional electron beam lithography into hydrogen silsesquioxane (HSQ) down to a width of 15-30 nm.
We present the single layer process fabrication and measurements of nanowires galvanically coupled to a superconducting lumped element microwave resonator.

TT 5.11 Mon 12:45 H22

Localized quantum phase slips in TiN nanowires — •Ina Schneider[1], Tatyana Baturina[1,2], and Christoph Strunk[1] — [1]Inst. f. Exp. und Angewandte Physik, Uni Regensburg — [2]Inst. f. Semiconductor Physics, RAS, Novosibirsk, Russia

We investigate TiN nanowires with 780 nm length and widths ranging from 50-780 nm close to the superconductor/insulator transition. In zero magnetic field the superconducting transition of wider wires resembles that of macroscopic films, while narrower wires develop a finite and T-independent resistance down to the lowest temperatures. In perpendicular magnetic field B a pronounced nonmontonic magnetoresistance occurs. The $R(T)$-curves at fixed B show a reentrant insulating behavior very similar to that of Coulomb-blockaded linear arrays of Josephson junctions [1].

The $I(V)$-characteristics display a characteristic cross-over from the dc-Josephson effect towards Coulomb blockade at very low voltages and temperatures within a globally superconductive-like $I(V)$. In the linear regime, the magnetoresistance displays strong fluctuations. We interpret our results in terms of disordered Josephson networks with a B-dependent Josephson coupling energy that favors coherent quantum phase slips at certain B.

[1] A. Ergül, et al., NJP **15**, 095014 (2014).

TT 6: Superconductivity: Properties and Electronic Structure

Time: Monday 10:00–13:00 Location: H19

TT 6.1 Mon 10:00 H19

Superconductivity in intercalated topological insulator $Tl_xBi_2Te_3$ — •Zhiwei Wang[1,2], Alexey A. Taskin[1,2], and Yoichi Ando[1,2] — [1]Institute of Physics II, University of Cologne, D-50937 Cologne, Germany — [2]Institute of Scientic and Industrial Research, Osaka University, Osaka 567-0047, Japan

Bulk superconductivity has been discovered in $Tl_xBi_2Te_3$, which is derived from the topological insulator Bi_2Te_3 by intercalating Tl. The superconducting volume fraction of up to 95% (determined from specific heat) with T_c of 2.28 K is obtained for samples with $x = 0.6$, where the carriers are p-type with the density of $\sim 1.8 \times 10^{20}$ cm^{-3}. The thermodynamic upper critical field B_{c2} obtained from specific heat presents a conventional temperature dependence with the zero-temperature-limit value of 1.06 T; however, resistive transitions under magnetic fields suggests a higher B_{c2}, which hints at an unconventional nature of the superconductivity. The temperature dependence of the specific heat in 0 T suggests that the superconducting state is fully gapped. This material is an interesting candidate of a topological superconductor which may be realized by the strong spin-orbit coupling inherent to topological insulators.

TT 6.2 Mon 10:15 H19

Vortex-bound zero-energy modes in the noncentrosymmetric superconductors — •Oleksiy Kashuba[1] and Carsten Timm[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Deutschland — [2]Institut für Theoretische Physik, TU Dresden, 01062 Dresden, Deutschland

Nodal noncentrosymmetric superconductors are known to be the candidate for the realization of the surface-bound zero-energy modes. We investigate whether the similar modes bound to the 1D defects may exist in the superconductors with unconventional pairing. The known example of such modes are the Majorana states in the half-integer vortices in the $p_x + ip_y$-wave superconductor. We showed that there is a precise mapping of the localized cylindrical solutions in the superconductor with arbitrary pairing onto the localized solutions in the superconducting Anderson chain model. We studied different superconductor pairing which depends on the crystal symmetry and found out that in some systems, like ones with cubic symmetry ($Li_2Pd_xPt_{3-x}$, Mo_3Al_2C), such states are forbidden, and for other, like ones with tetrahedral symmetry (Y_2C_3), the zero-energy states may exist.

TT 6.3 Mon 10:30 H19

Heat Capacity Measurements of Sr_2RuO_4 under uni-axial Strain — •You-sheng Li[1,2], Alexandra Gibbs[3], Clifford Hicks[1], Andrew Mackenzie[1,2], and Michael Nicklas[2] — [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 Sr_2RuO_4 is $p_x \pm ip_y$. By applying strain along ⟨100⟩-direction, the degeneracy of the p_x and p_y components is lifted, and thus there should be two critical temperatures (T_c). Hicks et al. [1] have observed an increase of T_c of Sr_2RuO_4 under both compressive and tensile strains, by measuring the susceptibility, which is sensitive only to the first transition. Their results also indicate, indirectly, that any splitting of T_cs might be small. For a direct test of possible splitting, we measure the heat capacity of Sr_2RuO_4 under strain. To do so, we are developing an approach to measure heat capacity under non-adiabatic conditions. We have observed an increase of T_c under compressive strain. This is the first thermodynamic evidence of the strain-induced increase in T_c of Sr_2RuO_4.

[1] C. W. Hicks et al., Science **344**, 283 (2014).

TT 6.4 Mon 10:45 H19

Sr_2RuO_4 at high uniaxial strain — •Alexander Steppke[1], Lishan Zhao[1,2], Clifford Hicks[1], Daniel Brodsky[1,2], Mark Barber[1,2], Alexandra Gibbs[3], Yoshiteru Maeno[4], and Andrew Mackenzie[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]University of St Andrews, UK — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany — [4]Kyoto University, Japan

We applied high anisotropic strains to high-quality single crystals of the superconductor Sr_2RuO_4, to gain information on the influence of anisotropic Fermi surface distortions on its superconductivity. Due to proximity to a van Hove singularity, one of the Fermi surfaces distorts particularly strongly in response to anisotropic strain [1]. The superconducting properties also vary strongly: we show susceptibility and resistivity data indicating that T_c more than doubles as strain is applied, and passes through a sharp peak. Similarly, the upper critical field H_{c2} for fields both parallel and perpendicular to the crystallographic c axis increases substantially. For fields perpendicular to the c axis, there is strongly hysteretic behaviour at low temperatures, that may be due to Pauli limiting.

[1] C. W. Hicks et al., Science **344**, 283 (2014)

TT 6.5 Mon 11:00 H19

$Cd_2Re_2O_7$: Temperature dependence of the superconducting order parameter and the effect of quasiparticle self-energy — F. S. Razavi[1], Y. Rohanizadegan[1], M. Hajialamdari[1], M. Reedyk[1], B. Mitrovic[1], and •R. K. Kremer[2] — [1]Department of Physics, Brock University, St. Catharines, ON L2S 3A1, Canada — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany

The temperature dependence and the magnitude of the superconducting order parameter of single crystals of $Cd_2Re_2O_7$ ($T_c = 1.02$ K) were measured using soft point-contact spectroscopy. The order parameter, $\Delta(T)$, increases steeply below the superconducting transition temperature and levels off below ~ 0.8 K at a value of 0.22(1) meV, about 40 % larger than the BCS value. Our findings indicate the presence of a strong electron-phonon interaction and an enhanced quasiparticle damping and may be related to a possible phase transition within the superconducting region at ~ 0.8 K. In order to fit the conductance spectra and to extract the order parameter at different temperatures we generalized the Blonder-Tinkham-Klapwijk theory by including the self-energy of the quasiparticles into the Bogoliubov equations. This modification enabled excellent fits of the conductance spectra.

15 min. break

TT 6.6 Mon 11:30 H19

Electronic structure determination of $R_3T_4Sn_{13}$ — •Xiaoye Chen[1], HongEn Tan[1], Lina E. Klintberg[1], Swee K. Goh[1,2], Sven Friedemann[1,3], Jinhu Yang[4,5], Bin Chen[4,5], Kazuyoshi Yoshimura[5], David A. Tompsett[1], Wing Chi Yu[2], F. Malte Grosche[1], and Michael Sutherland[1] — [1]University of Cambridge, Cavendish Laboratory, Cambridge, UK — [2]The Chinese University of Hong Kong, Department of Physics, Hong Kong, China — [3]University of Bristol, HH Wills Physics Laboratory, Bristol, UK — [4]Hangzhou Normal University, Department of Physics, Hangzhou, China — [5]Kyoto University, Department of Chemistry, Kyoto, Japan

The quasi-skutterudite superconducting material family $R_3T_4Sn_{13}$ (R = Ca, Sr, T = Ir, Rh) was recently shown to have a composition and pressure induced structural quantum phase transition. The end member material $Sr_3Ir_4Sn_{13}$ at ambient pressure and above T* = 147 K adopts a simple cubic structure (I phase, Pm-3n). Below this temperature, the compound enters the I* phase, thought to result from a superlattice distortion of the I phase with twice the original lattice constant. We compare our quantum oscillation data for $Sr_3Ir_4Sn_{13}$, measured at a wide range of angles, with DFT calculations for the I and I* phases, as well as other proposed possibilities such as merohedral twining domains. We complement this comparison with thermal conductivity measurements of other materials in the family to provide important insights into the nature of the superlattice distortion.

TT 6.7 Mon 11:45 H19

Correlating properties and microstructure of YBCO thin films by magnetic X-ray microscopy — •Stephen Ruoss[1], Claudia Stahl[1], Patrick Zahn[1,2], Jonas Bayer[1,2], Markus Weigand[1], Gisela Schütz[1], and Joachim Albrecht[2] — [1]Max-Planck-Institute for Intelligent Systems, Heisenbergstraße 3, 70569 Stuttgart — [2]Research Institute for Innovative Surfaces, FINO, Aalen University, Beethovenstraße 1, 73430 Aalen

The magnetic flux distribution in high-temperature superconductors namely YBCO has been observed using a novel high-resolution technique based on the X-ray magnetic circular dichroism (XMCD) [1,2]. Therefore, a CoFeB layer is deposited on the superconductor which exhibits a strong XMCD-effect. X-ray absorption measurements with circular polarized radiation allows the analysis of the magnetic flux distribution in the superconductor via the soft-magnetic sensor layer [3,4]. In the total electron yield (TEY) mode of the scanning X-ray microscope (SXM) the surface structure and the magnetic domains can be imaged at the same time. Having obtained such high resolution images, the correlation of magnetic flux penetration and defect structure of YBCO thin films can be analyzed.

The measurements have been performed at the scanning X-ray microscope MAXYMUS at Bessy II, HZB Berlin.

[1] S. Ruoß et al., APL **106**, 022601 (2015).
[2] C. Stahl et al., EPL **106**, 27002 (2014).
[3] C. Stahl et al., PRB **90**, 104515 (2014).
[4] C. Stahl et al., J. Appl. Phys. **117**, 17D109 (2015).

TT 6.8 Mon 12:00 H19

Superconducting properties of $La_{2-x}Ba_2CuO_4$ under pressure — •Wolf Schottenhamel[1], Markus Hücker[2], Anja Wolter-Giraud[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden, Germany — [2]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA

$La_{2-x}Ba_2CuO_4$ displays an anomalous doping dependence associated with a deep suppression of superconductivity at the hole concentration x=1/8. The so-called 1/8-anomaly is accompanied by a structural transition in the average rotational symmetry of the CuO_2 planes coinciding with the onset of a charge stripe order [1]. It has been claimed that static stripe order destroys the superconducting phase coherence, while dynamic stripe correlations may promote superconductivity. In order to achieve more information about the relationship between superconductivity, stripe order and crystal structure we performed magnetization measurements under pressure up to 3 GPa on the single crystalline $La_{2-x}Ba_2CuO_4$ with $0.095 \leq x \leq 0.125$. Moreover, we relate the magnetization data to pressure dependent X-Ray diffraction studies. This way, we show that the specific superconducting properties as function of pressure are clearly correlated to structural changes.

[1] M. Hücker *et al.*, PRB **83**, 104506 (2011)

TT 6.9 Mon 12:15 H19

The collapse of the columnar spatial topology of pseudogap excitations in the underdoped-overdoped transition of cuprate superconductors — •Jürgen Röhler — Universität zu Köln, 50937 Köln, Germany

The intensity I_{Q_0} of the $Q = 0$ nematic pseudogap excitations in $Bi_2Sr_2CaCu_2O_{8+x}$ was found to increase between $p \geq 0.06$ and 0.14 and to collapse at $p_{opt} = 0.16$, reaching zero at $p = 0.2$ [1]. Evidentally it maps the growth and the collapse of the bulge in the doping dependence of the basal-plane area (ab) of p-type cuprates [2]. The nematic topology of the pseudogap excitations results from the non-occupancy constraint for nn ZR-holes excluding $1a$ dimerization, but favoring $3a$ pair states with inequivalent $O_{x,y}$ sites. $3a$ pair states have hard core properties [3], yield d-type CDW excitations, and inflate the basal-plane area by a columnar topology against covalency-driven contraction. We show that optimal delocalization of ZR-holes at $p_{opt} = 1/6 \simeq 0.17$, tantamount to maximal connectedness of $3a$ pair states, will transform the columnar nematic pattern into isotropic tweedy striations, hence collapses I_{Q_0}, and the bulge.

[1] K. Fujita *et al.*, Science **344**, 612 (2015).
[2] J. Röhler, J. Superconductivity **17**, 159 (2004).
[3] J. Röhler, Int. Mod. Phys. **B19**, 255 (2005).

TT 6.10 Mon 12:30 H19

Trapped field measurements on MgB_2 bulk samples — Michael Koblischka[1], •Thomas Karwoth[1], XianLin Zeng[1], Kévin Berger[2], Bruno Douine[2], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, Saarland University, P. O. Box 151150, D-66041 Saarbrücken, Germany — [2]University of Lorraine, GREEN, 54506 Vandoeuvre-lès-Nancy, France

Trapped field measurements were performed on bulk, polycrystalline MgB_2 samples stemming from different sources with the emphasis to develop applications like superconducting permanent magnets ('supermagnets') and electric motors. We describe the setup for the trapped field measurements and the experimental procedure (field cooling, zero-field cooling, field sweep rates). The trapped field measurements were conducted using a cryocooling system to cool the bulk samples to the desired temperatures, and a low-loss cryostat equipped with a room-temperature bore and a maximum field of ±5 T was employed to provide the external magnetic field. The superconducting coil of this cryostat is operated using a bidirectional power supply. Various sweep rates of the external magnetic field ranging between 1 mT/s and 40 mT/s were used to generate the applied field. The measurements were performed with one sample and two samples stacked together. A maximum trapped field of 7 T was recorded. We discuss the results obtained and the problems arising due to flux jumping, which is often seen for the MgB_2 samples cooled to temperatures below 10 K.

TT 6.11 Mon 12:45 H19

High temperature superconductivity and flat bands in graphite: state of the art — Christian Precker[1], •Pablo Esquinazi[1], Ana Champi[2], Santiago Munoz[1], Jose Barzola-Quiquia[1], Israel Lorite[1], and Winfried Böhlmann[1] — [1]Division of Superconductivity and Magnetism, University of Leipzig, Linnéstraße 5, 04103 Leipzig, Germany — [2]Universidade Federal do ABC, Rua Santa Delia 166, 09210-170, Santo Andre, SP, Brazil

In this experimental work we studied the magneto-transport properties of natural graphite samples from a mine in Brazil. The reason for the study of these samples is the existence of well-defined, large 2D interfaces inside the samples. The observed huge magnetic field driven metal-insulator transition (MIT) is directly related to the existence of internal interfaces. Previous experimental results as well as theoretical work suggest the existence of granular superconductivity at certain interfaces between twisted Bernal stacking ordered regions or between rhombohedral and Bernal regions. We present results that indicate the existence of a transition in the electrical resistance at $T \gtrsim 320$ K. The observed irreversibility in the magnetoresistance at low magnetic fields and other transport details suggest the existence of superconducting paths at such high temperatures.

TT 7: Cold Atomic Gases

Time: Monday 10:15–13:00 Location: H18

TT 7.1 Mon 10:15 H18

Dimensional phase transition from 1D behavior to a 3D Bose-Einstein condensate — Denis Morath, Dominik Strassel, Axel Pelster, and •Sebastian Eggert — Department of Physics and Research Center Optimas, University Kaiserslautern, 67663 Kaiserslautern, Germany

The emergence of new properties from low-dimensional building blocks is a universal theme in different areas in physics. The investigation of transitions between isolated and coupled low-dimensional systems promises to reveal new phenomena and exotic phases. Interacting 1D bosons, which are coupled in a two-dimensional array, are maybe the most fundamental example of a system which illustrates the concept of a dimensional phase transition. However, recent experiments using ultracold gases have shown a surprising discrepancy between theory and experiment [1] and it is far from obvious if the power laws from the underlying 1D theory can predict the transition temperature and order parameter correctly for all interaction strengths. Using a combination of large-scale Quantum Monte-Carlo simulations and chain mean-field calculations, we show that the behavior of the ordering temperature as a function of inter-chain coupling strength does not follow a universal powerlaw, but also depends strongly on the filling.

[1] A. Vogler, R. Labouvie, G. Barontini, S. Eggert, V. Guarrera, and H. Ott, PRL **113**, 215301 (2014)

TT 7.2 Mon 10:30 H18

Interacting bosons on a two-leg ladder in the presence of gauge fields — Marie Piraud[1], Sebastian Greschner[2], •Fabian Heidrich-Meisner[1], Ian McCulloch[3], Temo Vekua[2], and Ulrich Schollwoeck[1] — [1]LMU Munich, Germany — [2]University of Hanover, Germany — [3]University of Queensland, Australia

We present the phase diagram of the Bose-Hubbard model on a two-leg ladder geometry in the presence of a homogeneous flux per plaquette, motivated by recent quantum gas experiments [1,2] that studied the regime of weak interactions. Based on extensive density matrix renormalization group simulations and a bosonization analysis, we explore the parameter space and calculate experimentally accessible observables. For hardcore bosons, the phase diagram comprises Meissner and vortex phases atop either superfluids or Mott insulators, depending on filling [4]. For moderate interactions, vortex lattices form at certain commensurate vortex densities. Very interestingly, the breaking of lattice translations in the vortex lattice phases can lead to a spontaneous reversal of the circulation direction of the chiral current [5].

[1] M. Atala et al., Nature Phys. **10**, 588 (2014)
[2] M. Mancini et al., Science **349**, 1510 (2015)
[3] B. K. Stuhl et al. Science **349**, 1514 (2015)
[4] M. Piraud et al., PRB **91**, 140406(R) (2015)
[5] S. Greschner et al., PRL **115**, 190402 (2015)

TT 7.3 Mon 10:45 H18

Sudden expansion and domain-wall melting of strongly interacting bosons in 2D optical lattices and on multileg ladders — •Johannes Hauschild[1], Frank Pollmann[1], and Fabian Heidrich-Meisner[2] — [1]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany — [2]Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, D-80333 München, Germany

We numerically investigate the expansion of clouds of hard-core bosons in a 2D square lattice using a matrix-product state based method. This non-equilibrium setup is induced by quenching the trapping potential to zero and is specifically motivated by recent experiments [1]. As the anisotropy of the amplitudes J_x and J_y for hopping in different spatial directions is varied from 1D to 2D, we observe a crossover from a fast ballistic expansion in the 1D limit $J_x \gg J_y$ to much slower dynamics in the isotropic 2D limit. We further compare the expansion of a cloud on multileg ladders and long cylinders with the melting of a domain wall and discuss the scenario of a condensation at finite momenta [2].

In addition, we study the domain-wall melting in the presence of a random on-site chemical potential. Tuning the inter-chain coupling J_y allows then to study the transition from an Anderson insulator in 1D to a many-body localized state in 2D.

[1] J. P. Ronzheimer et al., PRL **110**, 205301 (2013)
[2] J. Hauschild et al., PRA **92**, 053629 (2015)

TT 7.4 Mon 11:00 H18

Bosonic Self-Energy Functional Theory with Symmetry Breaking — •Dario Hügel[1], Philipp Werner[2], Lode Pollet[1], and Hugo U. R. Strand[2] — [1]Department of Physics, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstrasse 37, 80333 Munich, Germany — [2]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland

We derive a non-perturbative variational self-energy functional for symmetry-broken bosonic systems from the corresponding Baym-Kadanoff functional. The local physics of the Bose-Hubbard model in three dimensions, as well as its thermodynamical properties in two dimensions, can be accurately reproduced by searching for the stationary points of such a functional with respect to just three scalar variational parameters: a symmetry-breaking field, and the normal and anomalous components of an imaginary-time independent hybridization function. We further show how bosonic dynamical mean-field theory follows naturally from the self-energy functional when extending the formalism to an imaginary-time-dependent hybridization function, while the mean-field approximation is obtained when neglecting the contributions of non-condensed bosons.

The simplicity of the method makes studying more complex lattice boson systems tractable. In particular, it can be generalized to systems with synthetic gauge fields and spin-orbit interactions, where path integral Monte Carlo methods fail due to the notorious sign problem.

TT 7.5 Mon 11:15 H18

DMFT + NRG study of the SU(N) Fermi-Hubbard model — •Seung-Sup B. Lee, Jan von Delft, and Andreas Weichselbaum — Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, 80333 München, Germany

The SU(N) Fermi-Hubbard model, involving N flavors of fermions that interact fully symmetrically, has recently gained experimental relevance in the context of ultracold Ytterbium atoms in optical lattice, where the value of N can be changed controllably up to $N = 6$. The SU(2) Fermi-Hubbard model is well-known to exhibit a Mott metal-insulator transition, but a quantitative analysis of its SU(N)-symmetric counterpart has been limited so far to $N \leq 3$ or half-filling. Here we study the Mott transition of SU(N) Fermi-Hubbard model (up to $N = 6$) with dynamical mean-field theory (DMFT) using the numerical renormalization group (NRG) as impurity solver. By exploiting non-Abelian symmetry, the NRG yields the local spectral function efficiently with high spectral resolution over a wide range of system parameters, such as the interaction strength, chemical potential, and temperature.

15 min. break

TT 7.6 Mon 11:45 H18

Beyond the Hubbard bands in strongly correlated lattice bosons — •Hugo U. R. Strand[1], Martin Eckstein[2], and Philipp Werner[1] — [1]University of Fribourg, 1700 Fribourg, Switzerland — [2]Max Planck Research Department for Structural Dynamics, University of Hamburg-CFEL, 22761 Hamburg, Germany

We study the dynamics of the Bose-Hubbard model in- and out-of-equilibrium, using the real-time extension [1] of bosonic dynamical mean-field theory (BDMFT) [2] in combination with a Nambu strong-coupling impurity solver. Building on our previous study on quench dynamics [1], yielding qualitative agreement with cold-atom experiments [3], we here focus on theoretically reproducing and understanding cold-atom spectroscopy experiments [4, 5] in the strong-coupling limit. We perform non-equilibrium BDMFT interaction-modulation spectroscopy calculations, qualitatively reproducing experimental results, and explain the observed spectra by analyzing the structure of the equilibrium single-particle spectral function and the interaction-susceptibility. In particular, we discuss the nontrivial temperature dependence of the second resonance [6].

[1] Strand, Eckstein, Werner, PRX **5**, 011038 (2015)
[2] Anders, Werner, Troyer, Sigrist, Pollet, PRL **109**, 206401 (2012)

[3] Greiner, Mandel, Hansch, Bloch, Nature **419**, 51 (2002)
[4] Stöferle, Moritz, Schori, Köhl, Esslinger, PRL **92**, 130403 (2004)
[5] Clément, Fabbri, Fallani, Fort, Inguscio, PRL **102**, 155301 (2009)
[6] Strand, Eckstein, Werner, PRA **92**, 063602 (2015)

TT 7.7 Mon 12:00 H18

Competition between spin-selective localization and antiferromagnetism of correlated lattice fermions — •Jan Skolimowski[1], Dieter Vollhardt[2], and Krzysztof Byczuk[1] — [1]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, ul. Pasteura 5, PL-02-093 Warszawa, Poland — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135, Augsburg, Germany

Following our recent investigation of the paramagnetic ground state of correlated lattice fermions subjected to spin-dependent randomness [1], we study the magnetic ground state phase diagram of the Anderson-Hubbard model with spin-dependent disorder. The model is solved on a bipartite lattice within the dynamical mean-field theory with geometrically averaged local density of states, which makes our approach sensitive to Anderson localization and magnetic long range order. We determined the phase diagram which shows four phases: antiferromagnetic insulator, paramagnetic metal, and two distinct antiferromagnetic spin-selective localized phases. Our results show that antiferromagnetism (AF) is suppressed more strongly at weak spin-dependent disorder, whereas for large disorder strengths AF is sustained for all interaction strengths.

[1] J. Skolimowski, D. Vollhardt, K. Byczuk, PRB **92**, 094202 (2015)

TT 7.8 Mon 12:15 H18

Study of the Bose-Hubbard model with infinite-range interaction — •Jaromir Panas[1], Anna Kauch[2], and Krzysztof Byczuk[1] — [1]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warszawa, Poland — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 18221 Praha, Czech Republic

In relation to a recent experiment [1] we study the Bose-Hubbard model with an infinite-range interaction creating a staggered order. To this end we employ the bosonic dynamical mean-field theory (B-DMFT) [2] with a self-consistent, mean-field correction responsible for the exact treatment of an infinite-range interaction. The B-DMFT method is generalized to a system on a bipartite lattice. A self-consistent equation that includes effects of long-range ordering is presented. Comparison with experiment is achieved through a phase diagram. We find four distinct phases thus obtaining qualitative agreement with experimental results.

[1] R. Landig, L. Hruby, N. Dogra, M. Landini, R. Mottl, T. Donner, and T. Esslinger, arXiv:1511.00007.
[2] K. Byczuk, and D. Vollhardt, PRB **77**, 235106 (2008).

TT 7.9 Mon 12:30 H18

Semiclassical quantisation for a bosonic atom-molecule conversion system — Eva-Maria Graefe, •Alexander Rush, and Maria Graney — Imperial College, London, United Kingdom

In this talk I will consider a simple two state quantum model of atom-molecule conversion in cold atom systems, where bosonic atoms can combine into diatomic molecules and vice versa. The many-particle system can be expressed in terms of the generators of a deformed SU(2) algebra, and the mean-field dynamics takes place on a deformed version of the Bloch sphere resembling a teardrop, with a cusp singularity. I will demonstrate the mean-field and many-particle correspondence, showing how semiclassical methods can be used to recover features such as the many-particle spectrum from the mean-field description.

TT 7.10 Mon 12:45 H18

Frustrated magnetism with soft-shoulder potentials and cluster liquids — •Tao Ying[1,2], Marcello Dalmonte[3,4], and Guido Pupillo[1] — [1]IPCMS (UMR 7504) and ISIS (UMR 7006), University of Strasbourg and CNRS, 67000 Strasbourg, France — [2]Institute for Theoretical Solid State Physics, RWTH Aachen University, 52056 Aachen, Germany — [3]Institute for Theoretical Physics, University of Innsbruck, A-6020 Innsbruck, Austria — [4]Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, A-6020 Innsbruck, Austria

Cold bosonic atoms in optical lattices with finite-range soft-shoulder potentials (i.e., soft-core potentials with an additional hard-core on-site interaction) can cause cluster formation, which provides a natural source of frustration that leads to infinite ground state degeneracies, and hence to exotic quantum phenomena. Using quantum Monte Carlo simulations, we study the Bose-Hubbard model on a square lattice with soft-shoulder potentials V of finite-range $r_c = 2\sqrt{2}a$, where a denotes the lattice spacing. Upon increasing V/t, the model exhibits a superfluid to cluster liquid transition, where in the latter phase, the correlation functions such as the momentum distribution shows a distinct shape compared to the normal liquid. We also study the nature of the correlations and winding number histograms at the quantum critical point.

TT 8: Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Monday 10:15–13:00 Location: H21

TT 8.1 Mon 10:15 H21

Discovery of a new phase with magnetic short range correlations and its possible relevance for the hidden order in URu_2Si_2 — •Steffen Sykora[1] and Klaus W. Becker[2] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Technische Universität Dresden, D-01062 Dresden, Germany

In this paper we discuss a new phase of the Kondo lattice model which arises from the competition of Kondo and RKKY energy scales. Normally the Kondo lattice model is used to capture the low-energy physics of heavy fermion systems. However, according to the so-called Doniach picture the Kondo state will be replaced by an antiferromagnetic state for the case that the Kondo energy scale becomes smaller than the magnetic interaction between magnetic ions. In the present study we start instead from a modified electronic one-particle dispersion which avoids nesting of particle-hole excitations. Thus the magnetic ordered state should be suppressed which provides an opportunity for the inset of a new low-energy state with competing Kondo and magnetic energies. As will be shown, this new state avoids magnetic symmetry breaking but leads to a number of physical properties which are relevant for the understanding of the hidden order state in URu_2Si_2.

TT 8.2 Mon 10:30 H21

Effect of a magnetic moment on quantum spin Hall edge transport — •Florian Geissler[1], Jukka Väyrynen[2], and Leonid Glazman[2] — [1]Universität Würzburg, Würzburg, Germany — [2]Yale University, New Haven, USA

A local magnetic moment coupled to one dimensional helical transport channels, such as the edge states of a 2D quantum spin Hall insulator, can be a source of time-reversal invariant backscattering. We study the resulting correction to the conductance as a function of temperature T, dc bias voltage V and the repulsive electron-electron interactions characterized by the Luttinger liquid parameter $K < 1$. Such corrections display a characteristic power law dependence on V or T, with distinct scaling in the two regimes above and below the Kondo temperature, corresponding to the mechanisms of elastic and inelastic single-particle backscattering, respectively.

At energies above the Kondo temperature, the coupling to the magnetic moment can be considered weak. In this regime, if interactions are very small, $K \approx 1$, the correction to the conductance remains almost insensitive to V/T, even at high values of V/T. If electron interactions are more effective, $3/4 < K < 1$, this leads to corrections with small power law exponents below 1/2. Our findings agree with the experimental observation of a weak temperature dependence of the conductance in presumably weakly interacting QSH systems like HgTe and may further provide an alternative explanation for the recent experiment in more strongly correlated InAs/GaSb samples [1].

[1] Li et al., PRL **115**, 136804 (2015)).

TT 8.3 Mon 10:45 H21

The numerical renormalization group and symmetric multi-orbital models — •Andreas Weichselbaum[1], Katharina Stadler[1], Jan von Delft[1], Zhiping Yin[2], Gabriel Kotliar[2], and Andrew Mitchell[3] — [1]Ludwig Maximilians University, Mu-

nich, Germany — [2]Rutgers University, New Jersey, USA — [3]Utrecht University, The Netherlands

The numerical renormalization group (NRG) is a highly versatile and accurate method for the simulation of (effective) fermionic impurity models. Despite that the cost of NRG is exponential in the number of orbitals, by now, symmetric three-band calculations have become available on a routine level. [1] Here we present a recent detailed study on the spin-orbital separation in a three-band Hund metal with relevance for iron-pnictides via the dynamical mean field theory (DMFT). [2] In cases, finally, where the orbital symmetry is broken, we demonstrate that interleaved NRG [3] still offers an accurate alternative approach within the NRG with dramatically improved numerical efficiency at comparable accuracy relative to conventional NRG.

[1] A. Weichselbaum, Annals of Physics **327**, 2972 (2012)
[2] K. Stadler et al., PRL **115**, 136401 (2015)
[3] A. Mitchell et al., PRB **89**, 121105(R) (2014)

TT 8.4 Mon 11:00 H21

The path Integral formulation of the Schrieffer-Wolff transformation — •Farzaneh Zamani[1], Pedro Ribeiro[2], and Stefan Kirchner[3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]CeFEMA, Instituto Superior Tecnico, Universidade de Lisboa Avenida Rovisco Pais — [3]Center for Correlated Matter, Zhejiang University

The equivalence between the low-energy sector of the Anderson model in the so-called Kondo regime and the spin-isotropic Kondo model is usually established via a canonical transformation performed on the Hamiltonian, followed by a projection. Here, we present a path integral version of this important canonical transformation which relates the functional integral form of the partition function of the Anderson model to that of its effective low-energy model. The resulting functional integral assumes the form of a spin path integral and includes a geometric phase factor, i.e. a Berry phase. Our approach stresses the underlying symmetries of the model and allows for a straightforward generalization of the transformation to more involved models. It thus offers a systematic route of obtaining effective low-energy models and higher order corrections. We demonstrate the effectiveness of our approach by considering the charge Kondo model, and a quantum dot attached to magnetic leads.

TT 8.5 Mon 11:15 H21

Tailoring the magnetic ground state of a two-molecule Kondo system by chemical interactions — •Benedikt Lechtenberg[1], Taner Esat[3], Thorsten Deilmann[2], Christian Wagner[3], Peter Krüger[2], Ruslan Temirov[3], Michael Rohlfing[2], F. Stefan Tautz[3], and Frithjof B. Anders[1] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund — [2]Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich — [3]Institut für Festkörpertheorie, WWU Münster, 48149 Münster

We propose a novel approach for tailoring the magnetic properties of a nanostructure that relies on the ubiquitous non-magnetic chemical interaction between the constituents of the nanostructure instead of a magnetic exchange interaction. This is demonstrated in a dimer of metal-molecule complexes on the Au(111) surface: Changing the tunneling between both complexes, we tune the coupled dimer through a quantum phase transition from an underscreened Kondo doublet to a singlet ground state. In this talk, we explain the nature of the competing ground states and the role of parity breaking for the understanding of the STM spectra. Employing the results of a LDA calculation as a first principle input for a numerical renormalization group calculation, we are able to reproduce the experiment with excellent agreement.

15 min. break

TT 8.6 Mon 11:45 H21

Kondo effect in a carbon nanotube with spin-orbit interaction and valley mixing: A DM-NRG study — •Davide Mantelli[1], Catalin Pascu Moca[2,3], Gergely Zarand[2], and Milena Grifoni[1] — [1]Iunstitut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Deutschland — [2]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, HU-1521 Budapest, Hungary — [3]Department of Physics, University of Oradea, 410087 Oradea, Romania

We investigate the effects of spin-orbit interaction (SOI) and valley mixing on the transport and dynamical properties of a carbon nanotube (CNT) quantum dot in the Kondo regime. As these perturbations break the pseudo-spin symmetry in the CNT spectrum but preserve time-reversal symmetry, they induce a finite splitting Δ between formerly degenerate Kramers pairs. Correspondingly, a crossover from the SU(4) to the SU(2)-Kondo effect occurs as the strength of these symmetry breaking parameters is varied. Clear signatures of the crossover are discussed both at the level of the spectral function as well as of the conductance. In particular, we demonstrate numerically and support with scaling arguments that the Kondo temperature scales inversely with the splitting Δ in the crossover regime. In presence of a finite magnetic field, time reversal symmetry is also broken. We investigate the effects of both parallel and perpendicular fields (with respect to the tube's axis) and discuss the conditions under which Kondo revivals may be achieved.

TT 8.7 Mon 12:00 H21

Magnetic anisotropy in Shiba bound states across a quantum phase transition — •Nino Hatter[1], Benjamin W. Heinrich[1], Michael Ruby[1], José I. Pascual[2], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]CIC nanoGUNE and Ikerbasque, Basque Foundation for Science, Tolosa Hiribidea 78, Donostia-San Sebastian 20018, Spain

Magnetic adsorbates on a superconductor create a scattering potential for the quasi-particles of the superconductor. This leads to so-called Yu-Shiba-Rusinov (Shiba) states inside the superconducting gap and a Kondo resonance outside the gap.

We performed scanning tunneling microscopy and spectroscopy on paramagnetic manganese phthalocyanine molecules adsorbed on the type-I superconductor Pb. At 1.2 K we resolve triplets of Shiba resonances. A multitude of different adsorption sites provides access to a large range of magnetic coupling strengths with the substrate, which we use to identify the origin of the multiplets. We resolve the splitting of the Shiba states throughout the quantum phase transition from the "Kondo screened" to the "free spin" ground state and can link the splitting to the presence of magnetic anisotropy in the molecule-substrate system. Furthermore, the change in intensities of the Shiba resonances allows the unambiguous determination of the many-body ground and excited states.

TT 8.8 Mon 12:15 H21

Lindblad-Driven Discretized Leads for Non-Equilibrium Steady-State Transport in Quantum Impurity Models — •Frauke Schwarz[1], Moshe Goldstein[2], Andreas Weichselbaum[1], and Jan von Delft[1] — [1]Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, Munich — [2]Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv 6997801, Israel

The description of interacting quantum impurity models in steady-state non-equilibrium is an open challenge for computational many-particle methods: the numerical requirement of using a finite number of lead levels and the physical requirement of describing a truly open quantum system are seemingly incompatible. One possibility to bridge this gap is the use of additional continuous reservoirs coupled to the lead levels and represented by Lindblad terms in the Liouville equation [1]. Based on a simple scheme for the evaluation of Green's functions in quadratic Lindblad models, we discuss some important properties of this Lindblad approach. Moreover, we present first results on the single-impurity Anderson model out of equilibrium obtained within a matrix product state framework.

[1] A.A. Dzhioev, D. S. Kosov, J. Chem. Phys. **134**, 044121 (2011).

TT 8.9 Mon 12:30 H21

Tunneling processes into localized subgap states in superconductors — •Michael Ruby[1], Falko Pientka[1,2], Yang Peng[1,2], Benjamin W. Heinrich[1], Felix v. Oppen[1,2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany

The Yu-Shiba-Rusinov states bound by magnetic impurities in conventional s-wave superconductors are a simple model system for probing the competition between superconducting and magnetic correlations. Shiba states can be observed in scanning tunneling spectroscopy (STS) as a pair of resonances at positive and negative bias voltages in the superconducting gap. These resonances have been interpreted in terms of single-electron tunneling into the localized sub-gap states. This requires relaxation mechanisms that depopulate the state after an initial

tunneling event. Recently, theory suggests that the current can also be carried by Andreev processes which resonantly transfer a Cooper pair into the superconductor.

We performed high-resolution STS experiments on single adatom Shiba states on the superconductor Pb, and provide evidence for the existence of two transport regimes. The single-electron processes dominate at large tip-sample distances and small tunneling currents, whereas Andreev processes become important at stronger tunneling. Our conclusions are based on a careful comparison of experiment and theory.

TT 8.10 Mon 12:45 H21

Terahertz Spectroscopy of Kondo-Lattice Systems — •Christoph Wetli[1], Johann Kroha[2], Cornelius Krellner[3], Kristin Kliemt[3], Oliver Stockert[4], Hilbert v. Loehneysen[5], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]Institute of Physics, Bonn University — [3]Institute of Physics, Goethe University Frankfurt — [4]MPI for Chemical Physics of Solids, Dresden — [5]Institute of Solid State Physics, KIT

Quantum phase transitions are boosting the interest in the field of Kondo-lattice systems. Experimental insights have been mainly obtained by measuring the specific heat or the magnetic susceptibility and relating them to the increase of the quasiparticle effective mass. Lately, it has been demonstrated that ARPES experiments allow direct access to the electrons contributing to the Kondo-lattice effect. We show that THz radiation is a powerful and highly accurate alternative for investigating the approach to the coherent Kondo state of heavy-fermion systems. Photons in the THz range directly couple to the electronic heavy quasiparticles arising from the Kondo effect. This technique allows to study Kondo-lattice dynamics on the picosecond time scale. We report lifetime measurements of excited Kondo singlets for two crystalline rare earth heavy-fermion systems $CeCu_6$ and $YbRh_2Si_2$ and find that the lifetimes scale inversely with the Kondo temperature. THz spectroscopy thus gives a very different perspective towards the Kondo-lattice effect, with the unique ability to combine temporal resolution and possible measurements in magnetic field.

TT 9: Graphene: Structure and Dynamics (Joint session of DS, DY, HL, MA, O and TT organized by O)

Time: Monday 10:30–13:30 Location: H24

TT 9.1 Mon 10:30 H24

The electronic structure of graphene superlattices revisited — •Pilkwang Kim[1] and Cheol-Hwan Park[2] — [1]Department of Physics and Astronomy, Seoul National University, Seoul, Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul, Korea

We present the calculated electronic structure of graphene superlattices, which are graphenes under lateral, periodic potential. Previous studies on a graphene superlattice [1-3] have reported anisotropic group velocity renormalization, emergence of new zero-energy points, conductance resonance, etc. However, several features manifested in the electronic structure obtained from our numerical calculations, e.g., the movement of the Dirac points in momentum space, cannot be explained by the theories introduced in those studies. In this presentation, we discuss the reason why there are features in the electronic structure of graphene superlattices that were not captured by previous theories. We also discuss electronic structure obtained by using first- and higher-order perturbation calculations.

1.Park, C.-H., Yang, L., Son, Y.-W., Cohen, M. L. & Louie, S. G. New generation of massless Dirac fermions in graphene under external periodic potentials. Phys. Rev. Lett. 101, 126804 (2008). 2.Barbier, M., Vasilopoulos, P. & Peeters, F. M. Dirac electrons in a Kronig-Penney potential: Dispersion relation and transmission periodic in the strength of the barriers. Phys. Rev. B 80, 205415 (2009). 3.Brey, L. & Fertig, H. A. Emerging Zero Modes for Graphene in a Periodic Potential. Phys. Rev. Lett. 103, 046809 (2009).

TT 9.2 Mon 10:45 H24

Confinement effects in quasiparticle interference on epitaxial graphene nanoflakes — •Julia Tesch[1], Philipp Leicht[1], Felix Blumenschein[1], Tomas Löfwander[2], Luca Gragnaniello[1], and Mikhail Fonin[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Chalmers University of Technology, Göteborg, Sweden

In the search for suitable materials to be used in nanoscale electronic devices, graphene quantum dots, ribbons and flakes have attracted increased attention amongst researchers, as they allow for a combination of graphene's linear electronic dispersion relation with interesting physical phenomena arising from the size quantization of the structures.

We present a comprehensive study of epitaxial graphene nanoflakes on noble metal surfaces by means of low-temperature scanning tunneling microscopy and spectroscopy. The analysis of quasiparticle interference patterns produced by elastic scattering at defects allows for a clear identification of graphene-related contributions visible as ringlike *inter*- and *intravalley* features within the Fourier transform images [1]. Lateral electronic confinement within these elongated flakes gives rise to additional scattering intensity related to transitions between the flake's transverse modes [2]. Additionally, we discuss the influence of edge configuration, lattice symmetry breaking and quasiparticle lifetime on the scattering, by comparison of the experimental results with tight-binding calculations of realistic graphene nanoflakes.

[1] P. Leicht *et al.*, ACS Nano **8**, 3735 (2014); [2] A. Bergvall *et al.*, Phys. Rev. B **87**, 205431 (2013).

TT 9.3 Mon 11:00 H24

Electron interference in ballistic graphene nanoconstrictions — •Johannes Aprojanz[1], Jens Baringhaus[1], Mikkel Settnes[2], Stephen Power[2], Anti-Pekka Jauho[2], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Technical University of Denmark, DTU Nanotech, Center for Nanostructured Graphene (CNG), 2800 Kgs. Lyngby, Denmark

Graphene nanoconstrictions (GNCs) are a central building block of future carbon electronic devices. However, the synthesis of constrictions with well-defined edges is challenging. Here, we use the tip of a scanning tunneling microscope (STM) for the local etching of graphene, which allows to define GNCs with variable dimensions of down to 1 nm. The GNCs are etched into fully ballistic graphene nanoribbons hosted on the sidewalls of SiC mesa structures [1]. Due to the highly precise etching technique as well as the exceptional electronic quality of the graphene (e.g. mean free path $> 10\ \mu$m), this system is ideal to study coherent transport phenomena. Therefore, the transport characteristics of constrictions with various dimensions are recorded by means of a variable temperature 4-tip-STM. Electron interference at the abrupt graphene interfaces gives rise to characteristic conductance peaks and transport gaps. Their appearance is described by a tight-binding and recursive Green's function approach which especially highlights the robustness of the resonances features against temperature as well as disorder.

[1] Baringhaus et al., Nature **506**, 349 (2014)

TT 9.4 Mon 11:15 H24

Graphene on Ru(0001) as a playground for the studies of the graphene-metal interaction — Elena Voloshina[1], Nikolai Berdunov[2], and •Yuriy Dedkov[2,3] — [1]HU Berlin, Germany — [2]SPECS GmbH, Germany — [3]IHP Frankfurt (Oder), Germany

We employ a combination of surface science methods (ARPES, STM/STS, AFM) and DFT calculations for the studies of the lattice mismatched graphene-Ru interface. Our results demonstrate a site-selective interaction (*strong* vs *weak*) between graphene and metal in the moiré lattice. In these studies we show that graphene-*hills* in this structure can be used as an array of electro-mechanical elastic nano-resonantors with very high resonance frequency (in the THz range). On the next step we modify the graphene-Ru interaction via intercalation. Here the scanning probe microscopy and spectroscopy were used to study the crystallographic structure and electronic properties of the uniform free-standing graphene layers obtained by intercalation of oxygen monolayer in the *strongly* bonded graphene/Ru(0001) interface. Spectroscopic data show that such graphene layer is heavily *p*-doped with the Dirac point located at 552 meV above the Fermi level,

that corroborates our ARPES data. Experimental data are understood within DFT and the observed effects are in good agreement with the theoretical data.

Invited Talk TT 9.5 Mon 11:30 H24

Direct view on non-equilibrium carriers in graphene with time-resolved ARPES — •Isabella Gierz — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

The linear band structure of graphene bares great potential for optoelectronic applications ranging from Terahertz lasing to efficient light harvesting. We explore the response of the Dirac carriers in lightly hole-doped epitaxial graphene samples to three different excitation schemes: interband transitions for $\hbar\omega_{\mathrm{pump}} > 2\mu_{\mathrm{e}}$, free carrier absorption for $\hbar\omega_{\mathrm{pump}} < 2\mu_{\mathrm{e}}$, and resonant phonon excitation for $\hbar\omega_{\mathrm{pump}} = 200\,\mathrm{meV}$. Time- and angle-resolved photoemission spectroscopy (tr-ARPES) allows us to map the transient population of the Dirac cone in momentum space over a large energy window of several electron Volts down to arbitrarily small excitation energies.

We find a short-lived population-inverted state for interband excitation [1], a simple metallic relaxation behaviour for free carrier absorption [1], and indications for a transient enhancement of the electron-phonon coupling constant when resonantly driving the in-plane phonon in bilayer graphene [2]. Furthermore, by improving the temporal resolution to ∼10 fs, we were able to identify impact ionization as the primary thermalization channel within the first ∼25 fs [3].

[1] Gierz et al., Nature Materials 12, 1119 (2013)
[2] Gierz et al., PRL 114, 125503 (2015)
[3] Gierz et al., PRL 115, 086803 (2015)

TT 9.6 Mon 12:00 H24

Electronic properties of ytterbium interaction with graphene on Ir(111) — Hendrik Vita[1], •Stefan Böttcher[2], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]SPECS Surface Nano Analysis GmbH, Berlin, Germany

The intercalation of metals in between graphene monolayers and a substrate is interesting from several points of view, for example in order to understand the effect of symmetry lowering in the interaction of the metal states with the specific graphene π bands in the region of the "Dirac cone". Here we present a study of the intercalation of a rare earth metal, Yb, in between graphene and Ir(111). Ytterbium exhibits an s-type valence band, making it possible to compare the electronic structure to the widely studied cases of alkali metals used as intercalates in graphene intercalation compounds. Using core level spectroscopy we follow the deposition of Yb and the evolution of the intercalated phase. LEED studies show that the structural arrangement of the intercalated Yb thin film leads to a $(\sqrt{3}\times\sqrt{3})\mathrm{R}30°$ phase. Angle-resolved photoemission reveals that the interaction between the metal states and the graphene π band near the K point induces an extremely strong n-type doping. Hybridization-induced band gaps open in the π band at binding energies of 0.3 eV and 1.6 eV due to the interaction with the strongly localized metal $4f$ states. We compare our data with other weakly and strongly interacting intercalated metal layers.

TT 9.7 Mon 12:15 H24

Plasma-assisted CVD graphene synthesis and characterization on nickel substrates — •Patricia Pop-Ghe, Lisa Krückemeier, Nicolas Wöhrl, and Volker Buck — Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr, 1, 47057 Duisburg, Germany

This work presents the synthesis of graphene by plasma-assisted chemical vapour deposition on polycrystalline nickel foils. It is initiated by the comparison of the mechanisms in CVD and plasma-assisted CVD on a nickel substrate and focusses on the development of a growth model for both sides of the substrate within the experimental results. In detail, the differences in graphene growth at the front and at the back side of the substrate are investigated and correlated to specific influence factors. It is shown that growth mode as well as expansion and quality of graphene sheets can be adjusted by process temperature and time respectively since carbon solubility and diffusion in nickel both hold strong temperature and time dependencies. The strong time dependance of graphene growth is further indicative of a reconstructional nature of graphene formation, which is further discussed in the developed growth model. In addition the influence of the substrate is investigated by comparing results from graphene growth on polycrystalline nickel foils and nickel single crystal(111) substrates, as well as graphene on nickel (synthesized graphene) and silicon dioxide substrates (transferred graphene). Raman mappings are demonstrated to confirm the quality of the synthesized graphene.

TT 9.8 Mon 12:30 H24

Determination of the optical constants of graphene at the carbon K-edge by transmission spectroscopy — •Christine Jansing[1], Hans-Christoph Mertins[1], Andreas Gaupp[1], Andrey Sokolov[2], Markus Gilbert[1], Andreas Schümmer[1], Hud Wahab[3], Heiko Timmers[3], Suk-Ho Choi[4], and Dominik Legut[5] — [1]Münster University of Applied Sciences, Stegerwaldstr. 39, D-48565 Steinfurt — [2]HZB, Albert Einstein Str. 15, D-12489 Berlin — [3]University of New South Wales, Canberra, ACT 2600, Australia — [4]Kyung Hee University, Yongin 446-701, Korea — [5]IT4Innovations Center, VSB-Technical University of Ostrava, CZ-708 33 Ostrava, Czech Republic

The transmission of linearly polarized synchrotron radiation through quasi-free-standing graphene, supported by a Si3N4-membrane, has been measured across the carbon K-edge. From the measured absorption spectrum, that represents the imaginary part, the real part of the refractive index has been extracted via a Kramers-Kronig transformation. Based on these detailed optical parameters, reflection spectra have been simulated for linearly polarized soft x-ray light incident on graphene-metal systems. Importantly, the simulations include the interference of light reflected from graphene and from light reflected from the metallic substrate, respectively. In addition the optical constants are compared to the ones obtained by various density function theory calculations using single-electron framework as well as the more complex many-body approaches to the electronic structure of free-standing graphene.

TT 9.9 Mon 12:45 H24

Origins of contact resistance in graphene-metal edge-contacts — •Bernhard Kretz[1], Christian Søndergaard Pedersen[2], Daniele Stradi[2], Aran Garcia-Lekue[1,3], and Mads Brandbyge[2] — [1]Donostia International Physics Center, E-20018 San Sebastian, Spain — [2]Center for Nanostructured Graphene, DTU Nanotech, Tech. Uni. of Denmark, DK-2800 Kongens Lyngby, Denmark — [3]IKERBASQUE, Basque Foundation for Science, E-48013 Bilbao, Spain

The transport properties of graphene-metal contacts play an important role in the design of graphene-based devices. Recent studies demonstrate the advantages of the edge-contact geometry over conventional surface contacts.[1,2] However, significantly different conclusions are reached regarding the influence of the metal on the conductance properties of edge-contacts: while simulations indicate that the contact resistance is of the same order of magnitude for different metals,[2] experiments reveal a strong metal-dependence.[1] The possible origins of these discrepancies are explored by studying the transport properties of graphene edge-contacts with different metals, different edge conformations, terminations and adsorption distances. We employ a density functional theory (DFT) based non-equilibrium Green-function (NEGF) approach, using the TranSIESTA code. Our results will offer insights towards a better understanding of the conductance properties of graphene-metal contacts deviating from ideal interfaces.

[1] Wang et al. Science 342, 2013; Chu et al. ACS Nano 8, 2014
[2] Matsuda et al., J. Phys. Chem. C 114, 2010

TT 9.10 Mon 13:00 H24

Magnetically confined quantum dots in graphene revealed by scanning tunneling spectroscopy — •Nils Freitag[1], Peter Nemes-Incze[1], Larisa Chizova[2], Colin R. Woods[3], Roman V. Gorbachev[3], Yang Cao[3], Andre K. Geim[3], Kostya S. Novoselov[3], Florian Libisch[2], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen, Otto-Blumenthal Street, 52074 Aachen, Germany — [2]Institute for Theoretical Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria — [3]School of Physics & Astronomy, University of Manchester, Manchester, United Kingdom

Confining graphene's chiral massless charge carriers by carving out nano-structures to circumvent Klein-tunneling suffers from disordered edges, impeding the control of the quasi-relativistic particles. Here, we use the electrostatic potential of an STM tip in combination with an homogeneous magnetic field to confine electrons in graphene without edges[1]. The confinement becomes visible as a fourfold charging sequence at B>2T, as expected from valley and spin degeneracy. Up to 40 charging peaks are observed in the hole and electron sector with charging energies of 5-10meV. Characteristic spatial charging patterns

created by potential modulations of the commensurate G on BN are found[2].

[1] G. Giavaras and F. Nori, PRB 85, 165446 (2012)
[2] C. R. Woods et al., Nat. Phys. 10(6), 451-456 (2014)

TT 9.11 Mon 13:15 H24

Controling intramolecular Hydrogen-transfer by 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

The atomic level control of the electron transport has important advantages for many applications, such as molecular electronics, solar cells and sensors. Electron transport properties can be controlled by the intramolecular reaction which reshape the electronic configuration without any significant change in the conformation. The STM-induced tautomerization, i.e the interconversion between two isomers due to the migration of Hydrogen, was observed in the form of telegraphic noise. Several methods to control the intramolecular Hydrogen-transfer by changing the chemical environment of the molecule have been developed, such as locating adatoms or introducing defects. However, these affect the molecules only in the nm range. In this work, using the gate-tunable STM, we demonstrate a global control of the chemical environment of the substrate which results in the changing of the switching rate of the Hydrogen-transfer. The system we have used is a molecular network of phthalocyanine on graphene. Understanding and controlling the influence of the field-effect on the molecules, will be crucial for the construction of future molecular devices for energy and information usages.

TT 10: Focus Session: Single Particle Sources for Electronic Devices I (Joint session of HL and TT organized by HL)

Organizers: Rolf Haug (Universität Hannover) and Janine Splettstößer (Chalmers University)

Time: Monday 11:30–13:00 Location: H10

Invited Talk TT 10.1 Mon 11:30 H10

A clean single electron source using voltage pulses generating levitons. — •Christian Glattli — Nanoelectronics Group, Service de Physique de l'État Condensé CEA-Saclay, 91191 Gif-sur-Yvette, France

A simple approach to realize an on-demand electron soource is to apply a voltage pulse on a contact of the conductor such that the resulting current pulse injects a single charge in the conductor. At first sight, the idea seems too naive to produce something useful. However it appears that this procedure perfectly works [1]. More surprisingly it contains a rich physics: the generation of a new kind of excitation carrying a single particle: a leviton. The method was theoretically considered 20 years ago by L. Levitov and collaborators [2] who found that a voltage pulse with Lorentzian shape produces a minimal excitation, i.e. such that the number of excitations generated is not larger than the number of injected charges.

In this talk, I will present the recent experimental generation of levitons. I will also show electron quantum optics applications, reporting a two-leviton quantum interference experiment, the electrical analog of the Hong Ou Mandel experiment with photons which reveal perfect electron coherence. Finally using electron quantum tomography [3] an almost complete picture of the Leviton wave-function can be experimentally given.

[1] J. Dubois et al, Nature 502, 659-663 (2013).
[2] Levitov et al., J. Math. Phys. 37, 4845*4856 (1996).
[3] T. Jullien et al., Nature 514, 603*607 (2014)

TT 10.2 Mon 12:00 H10

Feedback Control of Waiting Times — •Tobias Brandes — TU Berlin, Institut für Theoretische Physik

Feedback control is known as a versatile tool for controlling quantum transport. So far most approaches deal with a control of stationary quantities (such as charge and heat currents). In this talk I will address the direct control of a temporal correlation function, the waiting time distribution, under feedback conditions. Within a simple transport model, I try to analyse possible connections to the thermodynamics of information and (with C. Emary) to optimal control theory.

TT 10.3 Mon 12:15 H10

Squeezing of shot noise using feedback controlled single-electron tunneling — •Timo Wagner[1], Johannes C. Bayer[1], Eddy P. Rugeramigabo[1], Philipp Strasberg[2], Tobias Brandes[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität, D-30167 Hannover, Germany — [2]Institut für Theoretische Physik, TU Berlin, D-10623 Berlin, Germany

Quantum feedback control has been studied intensively in quantum optics for a variety of different mechanism and systems [1]. Here we demonstrate the squeezing of shot noise in a quantum dot (QD) using an exclusively electronic feedback loop. Therefore the single-electron counting statistics [2, 3] is monitored in real-time with a coupled quantum point contact (QPC) and the deviation from a target rate is fed back periodically to speed up or slow down the process. With increasing feedback response we observe a stronger squeezing and faster freezing of the charge current fluctuations. The measurements confirm previous theoretical predictions [4] and show that the feedback loop is very robust even under stronger experimental restrictions. Our technique is analog to the generation of squeezed light with in-loop photodetection in quantum optics [1, 5].

[1] H. M. Wiseman, *Quantum Measurment and Control*, Cambridge University Press, Cambridge (2009)
[2] S. Gustavson, et al., Surf. Sci. Rep. 64, 191 (2009)
[3] N. Ubbelohde, et al., Nature. Com. 3, 612 (2012)
[4] T. Brandes, Phys. Rev. Lett. 105, 06060 (2010)
[5] S. Machida, Y. Yamamoto, Opt. Commun. 57, 290 (1986)

Invited Talk TT 10.4 Mon 12:30 H10

(De)coherence of single electron wavepackets in quantum Hall edge channels — •Erwann Bocquillon[1,2], Arthur Marguerite[2], Vincent Freulon[2], Jean-Marc Berroir[2], Bernard Plaçais[2], Antonella Cavanna[3], Yong Jin[3], and Gwendal Fève[2] — [1]Physikalisches Institut (EP3), Universität Würzburg, Würzburg, Germany — [2]Laboratoire Pierre Aigrain, Ecole Normale Supérieure, Paris, France — [3]Laboratoire de Photonique et Nanostructures, Marcoussis, France

The ballistic propagation of electronic waves along the quantum Hall edge channels of a two dimensional electron gas bears strong analogies with photon optics. Ballistic and one-dimensional propagation are provided by the chiral quantum Hall edge states and electronic beam splitters can be implemented using quantum point contacts. These analogies have inspired a whole set of experiments and provide an efficient tool to understand electronic propagation in quantum conductors.

In this talk, I will present how one can implement electron quantum optics experiments down to a single charge resolution using an on-demand single electron emitter. In particular, we generate two indistinguishable quasiparticles that we characterize via their interference on a beamsplitter in an electronic analogue of the Hong-Ou-Mandel experiment. The visibility of two-particle interferences reveals decoherence effects due to interactions with the environment, and especially with other co-propagating edge channels. These implementations of electron quantum optics experiments pave the way to more complex ones, such as the tomography of a single electron.

TT 11: Focus Session: Single Particle Sources for Electronic Devices II (Joint session of HL and TT organized by HL)

Organizers: Rolf Haug (Universität Hannover) and Janine Splettstößer (Chalmers University)

Time: Monday 14:45–18:45 Location: H10

Invited Talk TT 11.1 Mon 14:45 H10

Energy- and time-resolved detection of hot single-electron wave packets — •Masaya Kataoka — National Physical Laboratory, Hampton Road, Teddington, Middlesex TW11 0LW, UK

On-demand semiconductor single-electron sources such as mesoscopic capacitors [1] have enabled an electronic analogy of quantum optics experiments. In further development of this field, the presence of a Fermi sea can present a challenge, causing decoherence due to electron-electron interactions [2]. One solution would be to set electron paths in an intrinsic region, where the conduction-band electrons are absent.

We demonstrate long-range electron transport along depleted edges of a two-dimensional system. A stream of hot electrons are emitted from a quantum-dot pump at ˜100 meV above the Fermi energy. Due to a strong magnetic field applied, these electrons travel along the edge defined by shallow etching of the surface, while the background Fermi sea along the edge is depleted by a surface gate that covers the edge.

The transport of the hot-electron wave packets is investigated with energy- and time-resolved detectors [3]. We discuss the measurements of arrival-time distribution measurements with time resolution of < 5 ps, the measurements of edge-state velocity [4], a method to extend LO-phonon scattering length to > 0.5 mm, and how the timing of two-electron emission can be tuned by the shape of pump drive signal.

[1] G. Fève et al., Science 316, 1169 (2007).
[2] V. Freulon et al., Nat. Commun. 6, 6854 (2015).
[3] J. D. Fletcher et al., Phys. Rev. Lett. 111, 216807 (2013).
[4] M. Kataoka et al., arXiv:1512.02906v1.

TT 11.2 Mon 15:15 H10

Dopant controlled single electron pumping through a metallic quantum dot in silicon — •Tobias Wenz[1], Frank Hohls[1], Xavier Jehl[2], Sylvain Barraud[3], Girts Barinovs[4], Jevgeny Klochan[4], and Vyacheslavs Kashcheyevs[4] — [1]Physikalisch-Technische Bundesanstalt (PTB), 38116 Braunschweig, Germany — [2]University Grenoble Alpes and CEA-INAC, F-38000 Grenoble, France — [3]University Grenoble Alpes and CEA-Leti-Minatec, F-38000 Grenoble, France — [4]Faculty of Physics and Mathematics, University of Latvia, LV 1002 Riga, Latvia

Single electron pumps produce a quantized current by transferring an integer number of electrons n each cycle with a high frequency f, so that the current is $I = nef$ [1], where e is the electron charge, enabling a redefinition of the ampere by fixing the value of e. Commonly, single electron pumps utilize gate-defined quantum dots to create a quantized current. In this work, we investigate a silicon nanowire produced from an industrial CMOS process and take advantage of single phosphorus dopants located in both barriers of a gate-defined quantum dot. Due to their strongly localized potential wells, single dopants have large charging energies and sharp resonances that strongly influence the coupling of the main quantum dot to source and drain. By modulating the gates with suitable RF signals to switch the coupling on and off a quantized current can be generated. The operation principle can be modeled using simple assumptions and allows the study of dynamic effects in a coupled single dopant/metallic quantum dot system.

[1] Kaestner and Kashcheyevs, Rep. Prog. Phys. **78**, 103901 (2015)

Invited Talk TT 11.3 Mon 15:30 H10

The reabsorption effect with single-electron sources — •Géraldine Haack[1] and Michael Moskalets[2] — [1]University of Geneva, Switzerland — [2]University of Kharkiv, Ukraine

In the past years, ground-breaking experiments have been realised in quantum transport in generating single-electronic states [1]. Their controlled emission enables the investigation of fundamental quantum mechanical properties such as the coherence of these single-electron states [2], useful for quantum information purposes, and the realization of fermionic analogues of quantum optics experiments such as the Hanbury-Brown and Twiss and Hong-Ou-Mandel experiments [3].

In this talk, we show that the heat current enables us to gain crucial information about the shape of the single-particle states compared to the charge current. To this end, we investigate the reabsorption effect with two single-electron sources coupled in series [4]. While the charge current nullifies, we show that the energy carried by electron-hole pairs is enhanced by a factor 2. This can be explained by the time symmetry of the single-electron state. We finally discuss the validity of the Joule-Lenz law and the fluctuation-dissipation relation, when cavities emit electron-hole pairs and particles of the same kind.

[1] G. Fève et al., Science 316, 1169 (2007); N. Maire et al. , Appl. Phys. Lett. 92, 082112 (2008); J. Dubois et al., Nature 502, 659 (2013). [2] G. Haack, Phys. Rev. B 84, 081303 (2011); G. Haack et al., Phys. Rev. B 87, 201302 (2013). [3] E. Bocquillon et al., Phys. Rev. Lett. 108, 196803 (2012); E. Bocquillon et al., Science 339, 1054 (2013). [4] M. Moskalets et al., Phys. Rev. B 87, 125429 (2013).

TT 11.4 Mon 16:00 H10

Maxwell's demon in the quantum regime — •Gernot Schaller — TU Berlin, Institut für Theoretische Physik

Feedback control can be a useful tool to change the Full Counting Statistics of charges being transferred through a microscopic device. It can be used to suppress fluctuations of the current or to revert its direction e.g., against a potential gradient. The latter case is particularly interesting from a thermodynamic perspective. For an implicit modeling of the controller, this leads to an apparent violation of the second law that may be interpreted as a modification due to a Maxwell-type demon. In contrast, when the control becomes autonomous, i.e., when the controller is included in the thermodynamic description, these apparent paradoxes can be nicely resolved. I will illustrate this viewpoint for electronic transport through quantum dots. Interestingly, these concepts from stochastic thermodynamics can be generalized to true quantum systems, where the evolution of degenerate populations and coherences in the system energy eigenbasis is coupled.

30 min. Coffee break

Invited Talk TT 11.5 Mon 16:45 H10

Electronic states in a driven quantum contact — •Mihajlo Vanevic[1], Julien Gabelli[2], Wolfgang Belzig[3], and Bertrand Reulet[4] — [1]Department of Physics, University of Belgrade, Serbia — [2]Laboratoire de Physique des Solides, Univ. Paris-Sud, France — [3]Fachbereich Physik, Universität Konstanz, Germany — [4]Département de physique, Université de Sherbrooke, Canada

Minimal excitations in a voltage-driven quantum conductor are electrons excited above the Fermi level. Generation of these minimal excitation states requires carefully tailored Lorentzian voltage pulses carrying an integer number of charge quanta. However, a general time-dependent voltage excites both electrons and electron-hole pairs whose number and probability of creation depend on the shape and the amplitude of the drive. We have studied the many-body electronic state created by a general voltage drive and expressed it manifestly in terms of single-electron and electron-hole quasiparticle excitations. We have confirmed our theoretical predictions by probing the constituent quasiparticle states in a Hong-Ou-Mandel-type experiment on a tunnel junction. The knowledge of the many-body state opens a way of engineering the required time profile or energy distribution of single-electron and electron-hole excitations. Harmonic drive with ac amplitude smaller than dc voltage offset can be used to create single-electron states with a small admixture of electron-hole pairs.

TT 11.6 Mon 17:15 H10

Lissajous Rocking Ratchet: Realization in a Semiconductor Quantum Dot — •Sergey Platonov[1,2], Bernd Kästner[3], Hans W. Schumacher[3], Sigmund Kohler[4], and Stefan Ludwig[1,2] — [1]Center for NanoScience & Fakultät für Physik, LMU-Munich, 80539 München, Germany — [2]Paul-Drude-Institut für Festkörperphysik, Hausvogteiplatz 5-7 10117 Berlin, Germany — [3]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [4]Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain

Symmetries are a very important concept of physics - the most famous one being the CPT symmetry. Breaking symmetries often gives

rise to interesting effects and, in particular, breaking the time-reversal symmetry is a requirement for many applications such as information processing. Here we present such a concept based on a quantum dot (QD) electrostatically defined in a AlGaAs/GaAs heterostructure. We break time-reversal symmetry by periodically modulating its barriers such that a single electron tunneling current occurs. The current direction can be controlled by introducing a phase difference between the two periodic signals. We show that our QD resembles a Lissajous rocking ratchet. A consistent theoretical model based on scattering matrix formalism describes our experimental findings. Similar devices could be realized in a large variety of systems, for instance in nanomechanical or superconducting circuits. Possible applications include noise management, filtering and signal routing.

TT 11.7 Mon 17:30 H10

A charge-driven feedback loop in the resonance fluorescence of a single quantum dot — •Benjamin Merkel[1], Annika Kurzmann[1], Jan-Hindrik Schulze[2], André Strittmatter[2], Martin Geller[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstrasse 36, 10623 Berlin, Germany

Generating photons with transform-limited linewidths from semiconductor quantum dots (QDs) is challenging. Charge and spin noise from the environment cause spectral fluctuations of the resonance, limiting the generation of highly coherent photons.

In our micro-patterned samples we observe an electro-optical feedback mechanism by which the QD resonance frequency follows the excitation, leading to an optical bistability of the fluorescence signal. This feedback loop can be used to stabilize the resonance and reduce the noise of the emitted photons. We investigate the effect on InGaAs/GaAs QDs by time-resolved measurements of the fluorescence under two-colour excitation and also in a magnetic field. Experiments show a purely electrical origin of the feedback which lies in the formation of a hole gas at a valence band discontinuity close to the dot. The accumulated positive charge leads to a Stark shift of the dot's resonance frequencies. The hole gas is fed by carriers that are generated by resonant excitation of excitons in the dot and that tunnel into the hole gas states at the AlGaAs/GaAs interface. We are able to quantitatively reproduce the feedback dynamics by a numerical rate-equation model.

TT 11.8 Mon 17:45 H10

Exact duality for open system time-evolution and surprises in the heat current relaxation of an interacting quantum dot — •Roman Saptsov[1,2], Jens Schulenborg[3], Federica Haupt[4], Janine Splettstoesser[3], and Maarten Wegewijs[1,2,5] — [1]Institute for Theory of Statistical Physics, RWTH Aachen University, Aachen, Germany — [2]JARA - FIT — [3]Chalmers University of Thechnology, Götenborg, Sweden — [4]JARA Institute for Quantum Information, RWTH Aachen, Aachen, Germany — [5]Peter Grünberg Institut, FZ-Jülich, Jülich, Germany

Recent progress in nanoelectronics has brought the experimental detection and manipulation of few-electron heat currents in nanodevices within reach. However, a straightforward theoretical calculation of the heat-current relaxation – already for the simplest model of an Anderson quantum dot – exhibits a surprising behavior. More precisely, the contribution to the heat-current relaxation arising from the decay of the repulsive Coulomb interaction energy exhibits signatures of electron-electron attraction, and is governed by an interaction-independent decay rate [1]. The surprising behavior of the interaction-induced dissipation mode can only be understood with the help of a new duality relating the nonunitary evolution of an open quantum system to that of dual model with inverted energies [1]. Deriving from the fermion-parity superselection postulate, this duality applies to a large class of open systems, allowing for new general insights beyond the quantum-dot heat-current problem presented here.

[1] J.Schulenborg, R. B. Saptsov, F. Haupt, J. Splettstoesser, M.R. Wegewijs, arXiv: 1508.06145

TT 11.9 Mon 18:00 H10

Energy harvester with coupled quantum dots — •Holger Thierschmann[1,2], Rafael Sánchez[3], Börn Sothmann[4], Fabian Arnold[1], Christian Heyn[5], Wolfgang Hansen[5], Hartmut Buhmann[1], and Laurens W. Molenkamp[1] — [1]Experimentelle Physik 3, Universität Würzburg, Germany — [2]Kavli Institute of Nanoscience, Faculty of Applied Sciences, Delft University of Technology, The Netherlands — [3]Instituto de Cienca de Materiales de Madrid, CISC, Spain — [4]Département de Physique Theoretique, Univeristé de Genève, Switzerland — [5]Institute of Applied Physics, University of Hamburg, Germany

Multi-terminal thermoelectrics recieve an increasing attention because they allow for ways to separate heat and charge flow, thus pointing out a new route towards highly efficient thermoelectric devices. Here we present experiments on a three-terminal energy harvester with Coulomb coupled quantum dots (QD) following a recent proposal [1]. Energy is extracted from a hot electron reservoir via occupation fluctuations of a connected QD and is converted into a directed charge current in a conductor circuit which consists of another QD and two reservoirs at a lower temperature. Heat flow is mediated only through Coulomb interaction of the dots. The key ingredient of our device is an asymmetry in tunnel-coupling of the cold reservoirs and the QD which leads to rectification of charge fluctuations. Controlling this asymmetry with gate electrodes enables us to manipulate the direction of the resulting current even without changing the direction of heat flow. [1] R.Sánchez and M. Büttiker Phys. Rev. B 83 085428 (2011)

Invited Talk TT 11.10 Mon 18:15 H10

Clocked single-electron transfer: quantized currents and electron pair partitioning — •Frank Hohls — Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany

The clocked transfer of single electrons or electron pairs has applications both in metrology as quantized current source and in basic physics as building block for electron quantum optics. In the future redefinition of the International System of Units (SI), expected for 2018, the unit of the electrical current will be derived from a clock frequency f and the elementary charge e, $I = nef$. A promising realization is the non-adiabatic tunable-barrier pump which allows to transfer a highly quantized number of electrons n even at GHz driving frequency [1]. We will present latest results on accuracy verification of the resulting current quantization. For a pump driven at 545 MHz we find an agreement with $I = ef$ within the measurement uncertainty of 0.2 ppm [2]. Interestingly, the same type of electron pump also allows the controlled emission of electrons and electron pairs into a one-dimensional ballistic conductor formed at the edge of a quantum Hall system, opening the route to electron quantum optics experiments. We have examined the partitioning of such electrons at an electronic beam splitter using correlation measurements which validate high fidelity pair splitting and additionally reveal interesting correlation effects for the partitioning of electron pairs [3].

[1] B. Kaestner & V. Kashcheyevs, Rep. Prog. Phys. **78**, 103901 (2015).
[2] F. Stein *et al.*, Appl. Phys. Lett. **107**, 103501 (2015).
[3] N. Ubbelohde *et al.*, Nature Nanotechnol. **10**, 46 (2015).

TT 12: Graphene: Transport (Joint session of DS, DY, HL, MA, O and TT organized by HL)

Time: Monday 14:45–17:45 Location: H17

Invited Talk TT 12.1 Mon 14:45 H17

Advances in Raman Spectroscopy of Graphene and Layered Materials — •Andrea C. Ferrari — Cambridge Graphene Centre, University of Cambridge, Cambridge, CB3 OFA, UK

Raman spectroscopy is an integral part of graphene research [1]. It is used to determine the number and orientation of layers, the quality and types of edges, and the effects of perturbations, such as electric and magnetic fields, strain, doping, disorder and functional groups[2,3]. I will review the state of the art, future directions and open questions in Raman spectroscopy of graphene and related materials, focussing on the effect of disorder[3,4], doping[5,6] and deep UV laser excitation[7]. I will then consider the shear [8] and layer breathing modes(LBMs)[9],

due to relative motions of the planes, either perpendicular or parallel to their normal. These modes are present in all layered materials[10,11]. Their detection allows one to directly probe the interlayer interactions [10,11]. They can also be used to determine the elastic constants associated with these displacements: the shear and out-of-plane elastic moduli[12]. This paves the way to the use of Raman spectroscopy to uncover the interface coupling of two-dimensional hybrids and heterostructures[10-12].

1. A. C. Ferrari et al. Phys. Rev. Lett. 97, 187401 (2006) 2. A.C. Ferrari, D.M. Basko, Nature Nano. 8, 235 (2013) 3. A.C. Ferrari, J Robertson, Phys. Rev. B 61, 14095 (2000) 4. G. Cancado et al. Nano Lett. 11, 3190 (2011) 5. M. Bruna et al. ACS Nano 8, 7432 (2014) 6. A. Das et al. Nat. Nanotechnol. 3, 210 (2008) 7. A.C. Ferrari, S. Milana, P. H. Tan, D. M. Basko, P. Venezuela, submitted (2016) 8. P. H. Tan et al. Nature Materials 11, 294 (2012) 9. X. Zhang et al. Phys. Rev. B 87, 115413 (2013) 10. J. B. Wu et al. Nature Comms. 5, 5309 (2014) 11. J.B. Wu et al. ACS Nano, 9, 7440 (2015) 12. S. Milana et al. submitted (2016)

TT 12.2 Mon 15:15 H17

Landau Quantization in Twisted Bilayer Graphene — •Johannes C. Rode, Dmitri Smirnov, Christopher Belke, Hennrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

The bandstructure of bilayer graphene is highly sensitive to rotational mismatch between layers. At large angles, the twisted bilayer effectively behaves like two decoupled monolayers, while the dispersions merge in low-energy van Hove singurities for small interlayer twist[1]. Whereas the regime of large rotational mismatch has been extensively studied in transport experiments[2], there have been few reports on small angle samples[3,4] and none for the transition between the two angular regimes so far. We here examine the magnetotransport behavior across this transition, closing the gap in experimental evidence. The results are discussed with respect to theory[5] and and under special consideration of gate-induced layer asymmetries.

[1] Lopes dos Santos, J. M. B., Perez, N. M. R., Castro Neto, A. H. *Phys. Rev. Lett.* **99**, 25682.
[2] Schmidt, H. *et al. Appl. Phys. Lett.* **93**, 172108.
[3] Schmidt, H., Rode, J. C., Smirnov, D., and Haug, R. J. *Nat. Commun.* **5**, 5742.
[4] Lee, D. *et al. Phys. Rev. Lett.* **107**, 216602.
[5] de Gail, R., Goerbig, M. O., Guinea, F., Montambaux, G., Castro Neto, A. H. *Phys. Rev. B* **84**, 045436.

TT 12.3 Mon 15:30 H17

Magnetic exchange coupling across a graphene layer — •Alessandro Barla[1], Valerio Bellini[2], Stefano Rusponi[3], Paolo Ferriani[4], Marina Pivetta[3], Fabio Donati[3], François Patthey[3], Luca Persichetti[5], Sanjoy K. Mahatha[1], Marco Papagno[6], Cinthia Piamonteze[7], Simon Fichtner[4], Stefan Heinze[4], Pietro Gambardella[5], Harald Brune[3], and Carlo Carbone[1] — [1]Istituto di Struttura della Materia, CNR, I-34149 Trieste, Italy — [2]S3-Istituto di Nanoscienze-CNR, I-41125 Modena, Italy — [3]Institute of Condensed Matter Physics, EPFL, CH-1015 Lausanne, Switzerland — [4]Institute of Theoretical Physics and Astrophysics, University of Kiel, D-24098 Kiel, Germany — [5]Department of Materials, ETH Zürich, CH-8093 Zürich, Switzerland — [6]Dipartimento di Fisica, Universitá della Calabria, I-87036 Arcavacata di Rende, Italy — [7]Swiss Light Source, PSI, CH-5232 Villigen PSI, Switzerland

In order to access the potential of graphene in spintronic devices, its ability to mediate magnetic exchange interactions has to be verified. We present the results of our investigations of the magnetic coupling between Co atoms and Ni(111) mediated by epitaxial graphene. Experimental and theoretical calculations reveal that individual Co atoms occupy two distinct adsorption sites, with different magnetic coupling to the underlying Ni(111) surface. We further report a transition from an antiferromagnetic to a ferromagnetic coupling with increasing Co coverage. Our results highlight the extreme sensitivity of the exchange interaction mediated by graphene to the adsorption site and to the in-plane coordination of the magnetic atoms.

TT 12.4 Mon 15:45 H17

Transport studies in laterally density-modulated graphene-boron nitride-heterostructures — •Martin Drienovsky[1], Christian Baumgartner[1], Felix Simbürger[1], Takashi Taniguchi[3], Kenji Watanabe[3], Ming-Hao Liu[2], Fedor Tkatschenko[2], Klaus Richter[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik Universität Regensburg, 93053 Regensburg — [2]Institut für Theoretische Physik Universität Regensburg, 93053 Regensburg — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

We report on ballistic transport in graphene-boron nitride heterostructures with a tunable charge carrier density profile. Employing a dry van-der-Waals stacking method, we prepare high mobility graphene devices, where the charge carrier mean free path can exceed the lattice period of the induced multibarrier system by several times. These potential barriers are generated by multiple local top gate electrodes and a global back gate, and yield a pronounced Fabry-Pérot interference pattern in the bipolar transport regime. The extended ballistic length - in comparison to former samples - gets us within reach of the superlattice effect, which we highlight by matching the experimental data to a model calculation. We additionally apply a high, perpendicular magnetic field to our multibarrier systems and observe mode-mixing in the Quantum-Hall-regime of a 4-point measurement setup. By comparing samples with different top gate periods and separately controllable top electrodes, we study adiabatic and equilibrated unipolar edge channel transmission and suppression of equilibration at bipolar junctions.

15 min. Coffee Break

Invited Talk TT 12.5 Mon 16:15 H17

Thermodynamic picture of ultrafast conduction in graphene — •Dmitry Turchinovich[1], Zoltan Mics[1], Klaas-Jan Tielrooij[1,2], Ivan Ivanov[1], Xinliang Feng[1], Klaus Müllen[1], and Mischa Bonn[1] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]ICFO, 08860 Barcelona, Spain

Graphene has very high steady-state conductivity, which, however, does not hold in the regime of ultrafast, sub-picosecond electric fields corresponding to the terahertz (THz) frequencies. Here we show that in graphene, the electron conduction on an ultrafast timescale is determined by a simple thermodynamic balance maintained within its electronic system acting as a thermalized electron gas [1]. The energy of ultrafast electric currents passing trough graphene is near-instantaneously converted into the thermal energy of its entire charge carrier population, thereby raising the electronic temperature and reducing the chemical potential. The interplay between electron heating and cooling dynamics in graphene ultimately defines its ultrafast conductivity. We demonstrate that this simple thermodynamic picture describes very well the THz linear, nonlinear, and photo-induced conductivity of this remarkable material [1-3].

[1] Z. Mics, K.-J. Tielrooij, K. Parvez, S. A. Jensen, I. Ivanov, X. Feng, K. Müllen, M. Bonn, and D. Turchinovich, Nat. Commun. 6, 7655 (2015). [2] S. A. Jensen, Z. Mics, I. Ivanov, H. S. Varol, D. Turchinovich, F. H. L. Koppens, M. Bonn, and K. J. Tielrooij, Nano Lett. 14, 5839 (2014). [3] I. Ivanov, M. Bonn, Z. Mics, and D. Turchinovich, EPL - Europhys. Lett. 111, 67001 (2015).

TT 12.6 Mon 16:45 H17

Magnetotransport in graphene antidot arrays: semiclassics and moiré lattices — •Andreas Sandner[1], Tobias Preis[1], Christian Schell[1], Paula Giudici[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]NIMS, 1-1 Namiki, Tsukuba, Japan

Embedding graphene into a heterostructure with hexagonal boron nitride (hBN) on both sides was shown to be an efficient way of achieving a high bulk mobility. However, nanopatterning graphene can add extra damage and drastically degrade the intrinsic properties by edge disorder. But graphene encapsulated between hBN is protected during a top-down fabrication procedure. In this way, we can prepare graphene-based antidot lattices where the high mobility is preserved.

We performed magnetotransport experiments in monolayer-graphene antidot lattices with lattice periods down to 50 nm. We observe pronounced commensurability features in ρ_{xx} stemming from ballistic orbits around one or several antidots. Due to the short lattice period in our samples, we can explore the boundary between the semiclassical and the quantum transport regime, as the Fermi wavelength of the electrons approaches the smallest length scale of the artificial potential.

Additionally, we study the interplay between a moiré and the imposed antidot superlattice potential in several of our samples. There is a gradual suppression of the classical commensurability features by approaching the satellite Dirac points of the moiré potential.

TT 12.7 Mon 17:00 H17

Influence of disordered edges on transport properties in graphene — Dmitri Smirnov[1], Galina Yu. Vasileva[1,2,3], •Christopher Belke[1], Johannes C. Rode[1], Yurij B. Vasilev[2], Yurij L. Ivanov[2], and Rolf J. Haug[1] — [1]Institut fuer Festkoerperphysik, Leibniz Universitaet Hannover — [2]Ioffe Institute, Russian Academy of Sciences, St. Petersburg — [3]Peter the Great Polytech University, St. Petersburg

The influence of plasma etched edges on electrical transport and doping on graphene devices is studied. Mono- and bilayer samples were fabricated into a specific Hall bar geometry with differing width. The fabrication was done via transfer on a Si/SiO_2 substrate and structuring and contacting via plasma oxygen etching and e-beam lithography. The specific shape allows to investigate the influence of edge disorder on the overall doping and the effective mobility.
The doping concentration, calculated from the charge neutrality point, differs for every region and an inverse dependence on the region width was observed. The sample edge was determined as a strong p-doping source, dominating the bulk doping component and the edge doping contribution and efficiency was obtained.
A further study of the mobility for different regions was used to quantify the edge scattering. We find, that for decreasing region width the mobility decreases as well. This behavior can be attributed to the samples edge, establishing it as a further scattering mechanism.

TT 12.8 Mon 17:15 H17

Acoutoelectric currents in coated graphene on SiC — •Alberto Hernández-Mínguez, Abbes Taharoui, Marcelo Lopes, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Surface acoustic waves (SAWs) provide useful mechanisms for the dynamic modulation and transport of carriers in two-dimensional semiconductor heterostructures. In the case of graphene, we have recently shown that the piezoelectric fields accompanying SAWs can induce unipolar electric currents in lithographically patterned graphene layers grown on SiC. Due to the weak piezoelectricity of SiC, however, the interaction between SAW and carriers in graphene is relatively small. Future applications of the acoustic transport require the generation of strong SAWs for their efficient coupling to graphene, as well as the control of the density and type of carriers transported by the SAW. In this contribution, we study structures for efficient generation of high frequency acoustic transport (> 1 GHz) in graphene grown on SiC that are also compatible with top gates for the electric control of the carrier density. Several Rayleigh modes with frequencies up to 7 GHz are efficiently generated in our structure, inducing acoustic currents for the fundamental frequency that are 300 times larger than the ones reported in our previous devices. These results are an important step towards the dynamic control of carriers in graphene at the sub-micrometer regime, as well as for the dynamic manipulation of the electron spin by strain-induced gauge fields.

15 min. Coffee Break

TT 13: Transport: Topological Insulators - 2D (Joint session of DS, HL, MA, O and TT organized by TT)

Time: Monday 15:00–17:45 Location: H18

TT 13.1 Mon 15:00 H18

Probing the spin texture of generic helical edge states with an antidot — •Alexia Rod[1,2], Giacomo Dolcetto[1], Thomas L. Schmidt[1], and Stephan Rachel[2] — [1]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [2]Institut für Theoretische Physik, TU Dresden, Germany

Edge states of time-reversal topological insulators are generally described as helical edge states, where the spin-axis symmetry is conserved. However, this symmetry is usually not guaranteed in experimental realizations. In its absence, the most general model to describe edge states is called generic helical liquid. Using this framework, a rotation of the spin quantization axis has been predicted, independently of the microscopic model and of the considered geometry [1, 2].

Here we propose a scheme to probe the spin texture of the edge states on a transport device. We investigate the transport properties of generic helical edge states in a two-dimensional topological insulator bar with an antidot in its center. We show that the conductance is implicitly dependent of the spin texture in the case of uniform bulk or structural inversion asymmetry. We also study sequential tunneling and cotunneling in presence of Coulomb interaction due to electron confinement on the antidot.

[1] T.L. Schmidt, S. Rachel, F. von Oppen, L. Glazman, PRL **108**, 156402 (2012).
[2] A. Rod, T.L. Schmidt, S. Rachel, PRB **91**, 245112 (2015).

TT 13.2 Mon 15:15 H18

Electron quantum optics in 2d topological insulators — •Andrea Spichtinger, Sven Essert, Viktor Krückl, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Besides conventional quantum Hall systems [1], 2d topological insulators (TIs) are ideal systems providing ballistic channels for guiding charge carriers along edge states allowing for the study of two-particle interferometric effects. Employing wave-packet approaches we investigate correlations between indistinguishable spin pairs at opposite quantum spin Hall edges. Interconnecting opposite edges at TI constrictions or through quantum dots acting as "beam splitter" allows for realizing fermionic analogues of the famous photonic Hong-Ou-Mandel (HOM) effect. In particular, we will consider generalizations of the HOM effect since the dwell time of the quantum dot enters as a new timescale into HOM physics.

[1] E. Bocquillon et al., Ann. Phys. **526**, 1 (2014)

TT 13.3 Mon 15:30 H18

Transport in quantum spin Hall systems in parallel magnetic fields — •Michael Wimmer[1], Rafal Skolasinski[1], Dmitry Pikulin[2], and Jason Alicea[3] — [1]TU Delft, The Netherlands — [2]University of British Columbia, Canada — [3]Caltech, US

Edge states in quantum spin Hall (QSH) systems are protected by time-reversal symmetry, resulting in a qunatized conductance. A magnetic field breaks that protection, and should lead to a deviation from perfect quantization. We will discuss generic features of semiconductor-based QSH systems (such as HgTe/CdTe and InAs/GaSb) that affect the magnetic field dependence of edge state conductance, focusing on the effect of an in-plane field.

TT 13.4 Mon 15:45 H18

Spectral functions of the correlated topological insulator — •Damian Zdulski and Krzysztof Byczuk — Faculty of Physics, Institute of Theoretical Physics, University of Warsaw, ul.Pasteura 5, PL-02-093 Warsaw, Poland

In our recent paper [1], we have studied the influence of electron correlations on topological insulators (TIs) at finite temperatures. The correlated TI was represented by the Kane-Mele model with the interaction term as in the Falicov-Kimball model and it was examined within the Hartree and the Hubbard I approximations. In this talk, we will present extension of that analysis by investigating properties of the system within the dynamical mean field approximation. Our findings show that dynamical correlations yield totally new structures, which are seen in the the momentum dependent spectral functions. Namely, we see: 1) widening of Dirac nodes over finite range of **k** points in the Brillouin zone (BZ), 2) creation of almost flat subbands in a finite range of the BZ, 3) appearance of kinks, and 4) splitting of kinks with formation of overlapping bands.

[1] D. Zdulski, K. Byczuk, PRB **92**, 125102 (2015)

TT 13.5 Mon 16:00 H18

The topological Anderson insulator phase in the Kane-Mele model — Christoph P. Orth[1], •Tibor Sekera[1], Christoph Bruder[1], and Thomas L. Schmidt[2] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [2]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg

It has been proposed that adding disorder to a topologically trivial

mercury telluride/cadmium telluride (HgTe/CdTe) quantum well can induce a transition to a topologically nontrivial state. The resulting state was termed topological Anderson insulator and was found in computer simulations of the Bernevig-Hughes-Zhang model.

We show that the topological Anderson insulator is a more universal phenomenon and also appears in the Kane-Mele model of topological insulators on a honeycomb lattice. We numerically investigate the interplay between the parameters characterizing intrinsic spin-orbit coupling, extrinsic Rashba spin-orbit coupling and staggered sublattice potential. We establish the parameter regimes in which the topological Anderson insulator is found. For weak enough disorder, a calculation based on the lowest-order Born approximation reproduces the numerical data. Our results thus considerably increase the number of candidate materials for the topological Anderson insulator phase.

15 min. break

TT 13.6 Mon 16:30 H18

Interplay of topology and interactions in the quantum Hall regime of topological insulators: spontaneous symmetry breaking, tunable strongly interacting Luttinger liquid — •Stefan Jürgens, Maxim Kharitonov, and Björn Trauzettel — Institute of Theoretical Physics, University of Würzburg, Germany

We consider a class of two-dimensional topological insulators, in which the single-particle edge states are preserved in the presence of the magnetic field by a symmetry (such as crystalline) other than time-reversal, relevant to such materials as HgTe-type heterostructures.

We focus on the vicinity of the topological crossing point between two Landau levels. At half-filling, Coulomb interactions lead to the formation of the quantum Hall "ferromagnetic" many-body state with gapped charge excitations in the bulk. We derive and analyze the σ-model that describes the low-energy properties of this strongly interacting state, including the effect of the edge. We obtain the bulk phase diagram and find three phases, two with preserved and one with spontaneously broken U(1) symmetry. We study the collective edge charge excitations of these phases.

We demonstrate that in one of the phases with preserved U(1) symmetry, the edge charge excitations are gapless and described by a highly tunable, strongly interacting Luttinger liquid. When U(1) symmetry is broken in this phase, edge excitations become gapped and are described by a sine-Gordon model. Our main conclusion is that continuous U(1) symmetry is a necessary condition for the existence of the gapless edge excitations in this strongly interacting system.

TT 13.7 Mon 16:45 H18

Terahertz properties of Dirac electrons and holes in HgTe films with critical thickness — •Uladzislau Dziom[1], Alexey Shuvaev[1], Nikolai Mikhailov[2], Ze Don Kvon[2], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Novosibirsk State University, Novosibirsk 630090, Russia

We present and discuss properties of mercury telluride (HgTe) films with critical thickness in far-infrared (THz) spectral range. Density of charge carriers is controlled, using contact-free optical gating by visible light. Transmission measurements in applied magnetic field demonstrate switching from hole to electron-like behavior, as illumination time increases. The cyclotron mass of the electrons, extracted from the data, shows a square root dependence upon the charge concentration in a broad range of parameters. This can be interpreted as a clear proof of a linear dispersion relations, i.e. Dirac-type charge carriers.

TT 13.8 Mon 17:00 H18

Topological Edge States with Zero Hall Conductivity in a Dimerized Hofstadter Model — •Alexander Lau[1], Carmine Ortix[1,2], and Jeroen van den Brink[1,3] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [2]Institute for Theoretical Physics, Utrecht University, The Netherlands — [3]Department of Physics, TU Dresden, Germany

The Hofstadter model is one of the most celebrated models for the study of topological properties of matter and allows the study of the quantum Hall effect in a lattice system. Indeed, the Hofstadter Hamiltonian harbors the topological chiral edge states that are responsible for the quantized Hall conductivity.

Here, we show that a lattice dimerization in the Hofstadtermodel opens an energy gap at half-filling. What is more, we demonstrate that even if the ensuing insulator has a Chern number equal to zero, concomitantly a doublet of edge states appear that are pinned to specific momenta. We show that the presence of these states can be understood from the topological properties of lower dimensional cuts of the system, using a mapping of the Hofstadter Hamiltonian to a collection of one-dimensional Aubry-Andre-Harper (AAH) models. A sub-set of AAH chains in this collection preserve inversion symmetry. This guarantees the presence of topologically protected doublets of end modes to which the edge states are pinned. To explicitly prove the robustness of the emerging edge states, we define and calculate the topological invariant that protects them, which turns out to be an integer invariant for inversion-symmetric AAH models.

TT 13.9 Mon 17:15 H18

Disorder induced zero Landau level in topological insulator nanowires and its signature in conductance fluctuations — •Emmanouil Xypakis and Jens H Bardarson — Max-Planck-Institut f. Physik komplexer Systeme Noethnitzer Str. 38, 01187 Dresden, Germany

In this talk I will discuss the quantum transport properties of a disordered topological insulator in a strong magnetic field. The focus is on the case when the chemical potential is close to the Dirac point, where the transport is dominated by induced chiral modes. Disorder has a drastic role in the system electrical response by revealing a zero Landau level, which is absent for clean topological insulators. We study the dependence of the zero Landau level energy window on the system parameters, such as system size, disorder and magnetic field strength.

TT 13.10 Mon 17:30 H18

Time-resolved pure spin fractionalization and spin-charge separation in helical Luttinger liquid based devices — •Giacomo Dolcetto[1,2], Matteo Carrega[2], Alessio Calzona[2,3], and Maura Sassetti[2,3] — [1]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [2]SPIN-CNR, Genova, Italy — [3]Dipartimento di Fisica, Università di Genova, Italy

Helical Luttinger liquids, appearing at the edge of two-dimensional topological insulators, represent a new paradigm of one-dimensional systems, where peculiar quantum phenomena can be investigated [1]. Motivated by recent experiments on charge fractionalization [2], we propose a setup based on helical Luttinger liquids that allows one to time-resolve, in addition to charge fractionalization, also spin-charge separation and pure spin fractionalization. This is due to the combined presence of spin-momentum locking and interactions. We show that electric time-resolved measurements can reveal both charge and spin properties, avoiding the need of magnetic materials [3, 4]. Although challenging, the proposed setup could be achieved with present-day technologies, promoting helical liquids as interesting playgrounds to explore the effects of interactions in one dimension.

[1] G. Dolcetto, M. Sassetti, and T. L. Schmidt, arXiv preprint arXiv:1511.06141
[2] H. Kamata, N. Kumada, M. Hashisaka, K. Muraki, and T. Fujisawa, Nat. Nanotechnol. **9**, 177 (2014)
[3] A. Calzona, M. Carrega, G. Dolcetto, and M. Sassetti, Physica E **74**, 630 (2015)
[4] A. Calzona, M. Carrega, G. Dolcetto, and M. Sassetti, PRB **92**, 195414 (2015)

TT 14: Superconductivity: (General) Theory

Time: Monday 15:00–18:00 Location: H19

TT 14.1 Mon 15:00 H19

SCDFT, review and applications — •Antonio Sanna[1], Jose Flores-Livas[2], Arkady Davydov[1], Andy Linscheid[3], and E.K.U. Gross[1] — [1]Max Planck Institute of Microstructure Physics, Halle(Saale), Germany — [2]Department of Physics, Universität Basel, Switzerland — [3]Department of Physics, University of Florida, USA

We review the theoretical framework of Density Functional Theory for SuperConductors (SCDFT) and present recent applications and extensions as the calculation of the superconducting order parameter in real space[1]. SCDFT unlike conventional McMillan-Eliashberg theory, leads to reliable critical temperatures in a completely parameter free fashion. We discuss a formal connection between these approaches, the relative advantages and disadvantages, and how Eliashberg theory is used as ground for functional construction and to help extracting all the relevant physical properties from the solution of the SCDFT Kohn-Sham equations.

[1] A. Linscheid, A. Sanna, A. Floris, E.K.U. Gross, PRL **115**, 097002 (2015).

TT 14.2 Mon 15:15 H19

A novel approach in Eliashberg theory of superconductivity with ab-initio static and dynamic Coulomb interaction applicable for real materials — •Arkadiy Davydov, Antonio Sanna, Sangeeta Sharma, John Kay Dewhurst, and E. K. U. Gross — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

In standard Eliashberg methods the Coulomb interaction is usually restricted to the use of a single phenomenological parameter μ^* adjusted to give the right superconducting critical temperature (T_c). In this work we present a parameter-free Eliashberg approach, in which we treat the screened Coulomb interaction within the random phase approximation (RPA) in its static and full dynamic limit. The full energy range of the Coulomb interaction is taken into account, which becomes computationally affordable with the introduction of a suitable isotropic approximation. We have tested the method on a set of conventional superconductors. We will discuss the reliability of the predicted T_c both by using a static and a dynamic Coulomb interaction.

TT 14.3 Mon 15:30 H19

The role of Coulomb interaction for fluctuation corrections to the BCS theory of superconductivity — •Sonja Fischer and Jörg Schmalian — Institut für Theorie der Kondensierten Materie, KIT, Germany

We study fluctuation corrections to the gap equation of the BCS theory of superconductivity, taking into account the role of long ranged Coulomb interactions that is known to transfer superconducting phase fluctuations to the electron plasma frequency. Particular attention is paid to the previously discussed [1] cancellation of amplitude and phase fluctuation corrections in neutral superconductors.

[1] S. Kos A. J. Millis, and A. I. Larkin, PRB **70**, 214531 (2004)

TT 14.4 Mon 15:45 H19

Utilizing atomic force spectroscopy to test an alternative electrodynamic theory of superconductors — •Angelo Peronio and Franz J. Giessibl — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg, Germany

In the traditional theoretical description of superconductivity, a static electric field cannot penetrate a superconductor, since screening occurs like in a normal metal. This can be traced back to the fact that the London equations [1], the phenomenological equations describing the electrodynamics of superconductors, are derived within the Coulomb gauge. J. E. Hirsch proposes to use the Lorenz gauge instead [2], deriving a consistent solution where the electric field penetrates the superconductor up to the London penetration depth.

We report on initial experiments to test Hirsch's hypothesis, performed with a combined STM/AFM qPlus sensor equipped with a superconducting tip. If a superconductor screens electric fields differently from a normal metal, the electrostatic interaction between tip and sample should change when the tip becomes superconductive.

[1] F. London, Superfluids Vol. I, Wiley (1950)
[2] J. E. Hirsch, Physica C **508**, 21 (2015)

TT 14.5 Mon 16:00 H19

First-principles approach for superconducting slabs and heterostructures — •Gabor Csire — Wigner Research Centre for Physics, Budapest, Hungary

We present a fully ab-initio method to calculate the transition temperature for superconducting slabs and heterostuctures.

In the case of thin superconductor layers the electron-phonon interaction may change significantly. Therefore we calculate the layer dependent phonon spectrum to determine the layer dependence of the electron-phonon coupling for such systems. The phonon spectrum is than coupled to the Kohn-Sham-Bogoliubov-de Gennes equation via the McMillan-Hopfield parameter, and it is solved self-consistently.

The theory is applied to niobium slabs and niobium-gold heterostructures. Based on these calculations we investigate both the dependence of the superconducting transition temperature on the thickness of superconducting slabs and the inverse proximity effect observed in thin superconducting heterostructures.

TT 14.6 Mon 16:15 H19

Multiple scattering theory for superconducting heterostructures — •Balazs Ujfalussy — Wigner Research Centre for Physics, Budapest, Hungary

We generalize the screened Korringa-Kohn-Rostoker method for solving the corresponding Kohn-Sham-Bogoliubov-de Gennes equations for surfaces and interfaces.

As an application of the theory, we study the quasiparticle spectrum of Au overlayers on a Nb(100) host. We find that within the superconducting gap region, the quasiparticle spectrum consists of Andreev bound states with a dispersion which is closely connected to the underlying electronic structure of the overlayer. We also find that the spectrum has a strongly k-dependent induced gap. The properties of the gap are discussed in relation to the thickness of the overlayer, and it is shown that certain states do not participate in the Andreev scattering process.

From the thickness dependence of the gap size we calculate the superconducting critical temperature of Au/Nb(100) heterostructures what we compare with with experiments. Moreover, predictions are made for similar heterostructures of other compounds.

15 min. break

Invited Talk TT 14.7 Mon 16:45 H19

Spectroscopic signatures of collective modes in superconductors — •Lara Benfatto — ISC-CNR and Department of Physics, Sapienza University of Rome, Piazzale Aldo Moro 5, 00185, Rome, Italy

The technological progresses made in the last few years in the spectroscopic techniques require a critical revision of our understanding of the interactions of the light with the matter. In the case of superconducting systems light can in principle couple both to fermionic single-particle excitations and to bosonic superconducting collective modes, i.e. amplitude (Higgs) or phase fluctuations of the superconducting order parameter. At low temperature single-particle excitations are suppressed at energies below twice the gap value, leaving a window to the potential spectroscopic detection of the collective excitations in disordered superconductors. In this talk I will review some recent theoretical progresses in our understanding of the role of superconducting modes in linear and non-linear optical spectroscopy.

TT 14.8 Mon 17:15 H19

The Higgs-mode in charged superconductors without particle-hole symmetry — •Matthias Hecker — KIT, Karlsruhe

In a charged BCS superconductor there are two collective modes, namely the amplitude or Higgs mode and the plasmon mode reflecting the fact that due to long range Coulomb interactions phase fluctuations are shifted to the plasmon energy. Usually, the experimental determination of the Higgs mode is challenging as its energy sits right at the edge of the quasi-particle continuum. Using a field integral approach we investigate the possibility of detecting the Higgs mode by measuring density-density correlations. Without the assumption of particle-hole symmetry there is a finite coupling between the two excitation modes which is usually suppressed by the small factor $\frac{\Delta_0}{E_F}$.

However, in doped $SrTiO_3$ the latter ratio is of the order $\frac{\Delta_0}{E_F} \approx 10^{-1}$. We explore whether this coupling is sufficient to exploit the experimentally easy access to charge excitations in order to detect a Higgs mode signal.

TT 14.9 Mon 17:30 H19

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

New insights into the properties of the strongly correlated electron system can be gained by studying it in nonequilibrium. For instance, under the action of a strong laser pulse the system can undergo a phase transition and even the induced superconductivity may occur [1,2].

In this contribution we present a theoretical study of the nonequilibrium dynamics in the one-dimensional extended Hubbard model. Particular emphasis is on the possibility to induce superconductivity in this system driven out of equilibrium. Within the framework of the time-dependent Lanczos algorithm we investigate the time evolution of our model for two different nonequilibrium scenarios, which occur by (i) an interaction quench and by (ii) action of a light pulse. For both cases we calculate the time dependent optical conductivity and the superconducting correlation functions. In particular, we observe from our 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)
[2] D. Fausti et al., Science **331**, 189 (2011)

TT 14.10 Mon 17:45 H19

Unconventional superconductivity and interaction induced Fermi surface reconstruction in the two-dimensional Edwards model — •Dai-Ning Cho[1], Jeroen van den Brink[1], Holger Fehske[2], Klaus W. Becker[3], and Steffen Sykora[1] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, D-17487 Greifswald, Germany — [3]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany

We study the competition between unconventional superconducting pairing and charge density wave (CDW) formation for the two-dimensional Edwards Hamiltonian at half filling, a very general two-dimensional transport model in which fermionic charge carriers couple to a correlated background medium. Using the projective renormalization method we find that a strong renormalization of the original fermionic band causes a new hole-like Fermi surface to emerge nearby the center of the Brillouin zone, before it eventually gives rise to the formation of a charge density wave. On the new, disconnected parts of the Fermi surface superconductivity is induced with a sign-changing order parameter. We discuss these findings in the light of recent experiments on iron-based oxypnictide superconductors.

TT 15: Focus Session: Spectroscopy of Quantum Spin Liquids

The search for quantum spin liquids is a central endeavor in condensed matter and materials physics. It is motivated by their unusual nature, as they represent new phases of matter exhibiting topological forms of order not captured in the standard Landau-Ginzburg-Wilson picture, which includes fractionalized excitations and topologically protected edge modes. This session covers the central advances in the study of spin liquids over the last couple of years.

Organizers: Roderich Moessner and Frank Pollmann (MPI-PKS Dresden)

Time: Monday 15:00–17:45 Location: H20

Invited Talk TT 15.1 Mon 15:00 H20

Thermodynamics of Fractional Quantum Spin Liquids — •Yukitoshi Motome — University of Tokyo, Tokyo, Japan

After the proposal by P. W. Anderson in 1973, the quantum spin liquid (QSL) has attracted continuous interest as a new quantum state of matter. Although several candidate materials have been synthesized, it remains elusive to prove that their low-temperature state is a QSL, mainly because of the lack of order parameters that are experimentally accessible. On the other hand, one of the salient features of QSLs is the fractionalization of quantum spins. In this contribution, we theoretically show that the fractionalized spins manifest themselves in the finite-temperature properties, in particular, in the paramagnetic state as a precursor of QSL. We address this issue in the Kitaev model and its extensions, in which the quantum spin fractionalizes into two types of Majorana fermions in the QSL ground state. By using the newly-developed quantum Monte Carlo technique in the Majorana fermion representation, we find that many experimentally-accessible quantities experience the fractionalization in their temperature dependences. We also show that, in some cases, the fractionalization causes exotic phase transitions between the three states of matter in magnets: solid (long-range ordered state), gas (paramagnet), and liquid (QSL). Our findings will be helpful as "smoking gun" experiments for QSLs.

This work has been done in collaboration with J. Nasu, M. Udagawa, Y. Kamiya, and Y. Kato.

References at www.motome-lab.t.u-tokyo.ac.jp/publication-e.html.

Invited Talk TT 15.2 Mon 15:30 H20

Proximate Kitaev quantum spin liquid behavior in α-$RuCl_3$ — •Stephen Nagler — Quantum Condensed Matter Division, Oak Ridge National Laboratory

The magnetic semiconductor α-$RuCl_3$ is composed of very weakly coupled honeycomb layers of edge-sharing $RuCl_6$ octahedra. The Ru^{3+} ion has 5d electrons in a low spin state, and the system is expected to have an effective J = 1/2 single ion ground state with an interacting spin Hamiltonian containing Kitaev-like terms. Inelastic neutron scattering on powders and single crystals has been used to determine the energy scale of the magnetic interactions and the overall form of the magnetic fluctuations. The results indicate that the Kitaev term is significant. Moreover, detailed measurements of the response show evidence for the fractionalized excitations that are characteristic of the Kitaev Quantum Spin-liquid.

Research using ORNL neutron scattering facilities is supported by the US Department of Energy, Division of Scientific User Facilities.

Invited Talk TT 15.3 Mon 16:00 H20

Kagome chiral spin liquid and symmetry protected topological phases — •Yin-Chen He — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187, Dresden, Germany

In my talk I will introduce the chiral spin liquid phase that occurs in kagome antiferromagnets and discuss its physical origin as a gauged U(1) SPT phase. I will first present our numerical (DMRG) study on the kagome XXZ spin model that exhibits two distinct spin liquid phases, namely the chiral spin liquid and the kagome spin liquid (the groundstate of the nearest neighbor kagome Heisenberg model). Both phases extend from the extreme easy-axis limit, through SU(2) symmetric point, to the pure easy-plane limit. The two phases are separated by a continuous phase transition. Motivated by these numerical results, I will then focus on the easy-axis kagome spin system, and reformulate it as a lattice gauge model. Such formulation enables us to achieve a controlled theoretical description for the spin liquid phase. We then show that the chiral spin liquid is indeed a gauged U(1) symmetry protected topological (SPT) phase.

[1] Yin-Chen He, S. Bhattacharjee, F. Pollmann, and R. Moessner, arXiv:1509.03070
[2] Yin-Chen He, S. Bhattacharjee, R. Moessner, and Frank Pollmann, PRL **115**, 116803 (2015)
[3] Yin-Chen He and Yan Chen, PRL **114**, 037201 (2015).
[4] Yin-Chen He, D. N. Sheng and Y. Chen, PRL **112**, 137202 (2014).

15 min. break

Invited Talk TT 15.4 Mon 16:45 H20

Three-dimensional Kitaev spin liquids — •Maria Hermanns, Kevin O'Brien, Achim Rosch, and Simon Trebst — Institute for Theoretical Physics, Cologne, Germany

The Kitaev honeycomb model has become one of the archetypal examples of topological phases of matter. Being one of the few highly frustrated spin models that are exactly solvable, it has shaped our understanding of quantum spin liquid phases in general.

In this talk, we discuss the rich physics arising in generalizations of the Kitaev model to three-dimensional lattice structures. These models have low-energy degrees of freedom that are Majorana fermions, and that in general form metallic states. Depending on the underlying lattice structure, these can be (almost) conventional metals with a Majorana Fermi surface or Dirac semi-metals, where the gapless modes form Fermi lines or even Weyl nodes. The resulting quantum spin liquids differ not only in their experimental signatures, but also in their response to perturbations, such as an external magnetic field or additional interactions.

Invited Talk TT 15.5 Mon 17:15 H20

Landau levels of Majorana fermions in a spin liquid — •Matthias Vojta — Technische Universität Dresden, Germany

Majorana fermions, originally proposed as elementary particles acting as their own antiparticles, can be realized in condensed-matter systems as emergent quasiparticles, a situation often accompanied by topological order. Here we propose a physical system which realizes Landau levels - highly degenerate single-particle states usually resulting from an orbital magnetic field acting on charged particles - for Majorana fermions. This is achieved in a variant of a quantum spin system due to Kitaev which is distorted by triaxial strain. This strained Kitaev model displays a spin-liquid phase with charge-neutral Majorana-fermion excitations whose spectrum corresponds to that of Landau levels, here arising from a tailored pseudo-magnetic field. We show that measuring the dynamic spin susceptibility reveals the Landau-level structure by a remarkable mechanism of probe-induced bound-state formation.

TT 16: Transport: Quantum Dots, Quantum Wires, Point Contacts

Time: Monday 15:00–17:45 Location: H21

TT 16.1 Mon 15:00 H21

Suppression and break-down of Kondo screening in asymmetric double-quantum-dot systems — •Ammar Nejati, Katinka Ballmann, and Johann Kroha — Physikalisches Institut and Bethe Center for Theoretical Physics, Universität Bonn, Germany

Due to recent advances in semiconductor device technology, it is possible to investigate the Kondo effect in presence of magnetic correlations with fully-controllable double-quantum-dot (qdot) systems. Here we present a renormalization group (RG) method which can describe the different regimes observed in a highly-tunable semiconductor device with 2 qdots coupled to 3 leads ; especially, the principal observation which was the formation of a Kondo state for one qdot along with suppression of the Kondo resonance in the other, in presence of RKKY exchange interaction. The RG method is developed to consider local spin screening in multi-impurity Kondo systems in presence of magnetic fluctuations due to the carrier-mediated RKKY interaction. We calculate the beta-function for the Kondo coupling J between a localized spin (of the impurity/qdot) and conduction electrons in 1-loop order, taking into account that J is modified by the RKKY coupling to the neighbouring impurities/qdots. This leads to a suppression of T_K as a function of the dimensionless RKKY coupling parameter y, and ultimately, break-down of Kondo screening at a maximal RKKY coupling y_{max} which depends on the bare parametres only. In the 2-impurity case, the dependence of the renormalized Kondo temperature of each dot is drastically different if there is an asymmetry in the bare Kondo couplings.

TT 16.2 Mon 15:15 H21

Signatures of nonlocal Cooper pair transport in the critical current of a double dot Josephson junction — •Benedikt Probst[1], Fernando Domínguez[2], Alexander Schroer[1], Alfredo Levy Yeyati[2], and Patrik Recher[1,3] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Condensed Matter Physics Center (IFIMAC), and Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Laboratory for Emerging Nanometrology Braunschweig, D-38106 Braunschweig, Germany

We study the critical Josephson current flowing through a double quantum dot weakly coupled to two superconducting leads. We use analytical as well as numerical methods to investigate this setup in the entire range of its microscopic parameters, where we account for on-site interactions exactly. The characteristic behavior we find does not rely on a tunable magnetic field through the structure. Instead, we identify groundstate transitions as the unifying mechanism which gives rise to the rich phenomenology we observe, and which provide clear indications of nonlocal spin-entangled pairs that are consistent with recent experiments [1].

[1] S. Deacon *et al.*, Nat. Commun. **6**, 7446 (2015)

TT 16.3 Mon 15:30 H21

Current cross-correlations in double quantum dot Cooper pair splitter. — •Kacper Wrześniewski, Piotr Trocha, and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University, 61-614 Poznań, Poland

We investigate theoretically transport properties of a quantum dot (QD) system working as a Cooper pair splitter.[1] The device is coupled to one superconducting and two ferromagnetic leads. Presented results are calculated using real-time diagrammatic technique in the sequential tunneling approximation with respect to the coupling to ferromagnetic leads. The transport properties are evaluated within the superconductor subgap regime taking into account Andreev reflection processes solely.[2]

We focus on the analysis of current and current cross-correlations, both in linear and nonlinear responses. Current cross-correlations give additional information about dynamics of transport processes. We identify both positive and negative signs of current cross-correlations and discuss mechanisms leading to those results. Strong negative cross-correlations are found when the occupation number of QD system becomes degenerate and near the emergence of the triplet blockade, while positive ones occur in the most range where current flows due to crossed Andreev processes. Finally, we consider ferromagnetic leads polarization and temperature influences on aforementioned features.

[1] L. Hofstetter, S. Csonka, J. Nygård, and C. Schönenberger, Nature **461**, 960 (2009).
[2] P. Trocha and I. Weymann, PRB **91**, 235424 (2015).

TT 16.4 Mon 15:45 H21

Odd triplet superconductivity in ultrasmall quantum dots — •Stephan Weiss[1], Björn Sothmann[2], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg-Essen & CENIDE — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg

We report on the possibility to create odd frequency Cooper pairs in proximized interacting quantum dots attached to ferromagnetic leads. Spin blockade effects together with induced superconductivity allow electron pairs with same spin at different times to carry superconducting correlations. Besides the conventional finite singlet pairing amplitude on the dot, only odd frequency triplet pairing is possible here. This is in contrast to the double dot case [1]. We demonstrate how the order parameter for odd-frequency triplet pairing as well as the differential Andreev conductance are influenced when tuning gate and/or bias voltages, the angle of magnetizations of the leads and the coupling to the nearby superconductor.

[1] B. Sothmann, S. Weiss, M. Governale and J. König, PRB **90**, 220501 (2014).

TT 16.5 Mon 16:00 H21

Dynamical Properties of the 0.7-Anomaly in Quantum Point Contacts — •Dennis Schimmel and Jan von Delft — Ludwig-Maximilians-Universitaet Muenchen, Arnold-Sommerfeld-Center for theoretical physics

The 0.7-anomaly in the first conductance step of a quantum point contact is believed to arise from an interplay of geometry, spin dynamics and interaction effects. Previously [Bauer2014] it was shown that a one-dimensional tight-binding model with short-range interactions of intermediate strength reproduces the characteristic phenomenology of the 0.7-anomaly for the linear conductance at zero temperature and in equilibrium. Within these studies static quantities were computed using the functional renormalization group (fRG), formulated in terms of imaginary (Matsubara) frequencies. To gain access to real-frequency properties, we have formulated our fRG-scheme on the Keldysh-contour and used it to calculate dynamical quantities of a QPC, such as the local density of states, dynamical spin correlation functions, and transmission times. We have also used our Keldysh-fRG scheme to study the nonlinear conductance for a small bias voltage and discuss the effects of interactions on non-equilibrium transport.

15 min. break

TT 16.6 Mon 16:30 H21

Gauge freedom in pumping: interaction-induced geometric phases, adiabatic-response, and counting statistics — •Thilo Plücker[1], Maarten Wegewijs[2], and Janine Splettstoesser[3] — [1]Institute for Quantum Information, RWTH Aachen, 52056 Aachen, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, SE-41298 Göteborg, Sweden

In open quantum systems, adiabatic transport of various quantities such as charge, spin or energy can be realized by the slow and cyclic variation of two or more system parameters. An interesting example is offered by a quantum dot coupled to electrodes. Modulating in time its prime control parameters - the gate and bias voltage - a pumping current is generated, which is entirely due to the strong onsite Coulomb interaction [1].

In this contribution, we will show how to identify the geometric nature of this interaction-induced pumping of various quantities as a consequence of a generic gauge freedom of observables in open quantum systems using Landsberg's approach [2] to dissipative systems with symmetry. We present a general adiabatic pumping formula that shows that any interacting multilevel quantum dot in the wide-band limit exhibits an interaction-induced geometric phase. Our approach also sheds new light on Sinitsyn's [3] counting statistics approach to pumping.

[1] F. Reckermann, J. Splettstoesser, and Maarten R. Wegewijs, PRL **104**, 226803 (2010)
[2] A. S. Landsberg, PRL **69**, 865 (1992)
[3] N. A. Sinitsyn, J. Phys. A **42**, 193001 (2009)

TT 16.7 Mon 16:45 H21

Gate-tunable Andreev bound states in InSb Nanowire Josephson junction — •Ning Kang[1], Sen Li[1], Dingxun Fan[1], Philippe Caroff[2], and Hongqi Xu[1] — [1]Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, P. R. China. — [2]Division of Solid State Physics, Lund University, P. O. Box 118, S-221 00 Lund, Sweden

Hybrid InSb nanowire-superconductor devices are promising candidates for investigating Majorana modes in solid-state devices and future technologies of topological quantum manipulation. Here, we report low-temperature transport measurements on an individual InSb nanowire quantum dot coupled to superconducting contacts that exhibit an interplay between the Kondo effects and uperconductivity. We observed two types of subgap resonance states within the superconudcting gap, which can be attributed to gate-tunable Andreev bound states in Coulomb valleys with different Kondo temperatures. The presence of the gate-tunable 0 and pijunction allow us to invetigate the fundamental 0- pi transition. Detailed magnetic field and temperature evolution of level spectroscopy demonstrate different behavior of two types of the Andreev bound states. Our results exhibit that the InSb nanowires can provide a promising platform for exploring phase coherence transport and the effect of spin-orbit couping in semiconductor nanowire-superconductor hybird device.

TT 16.8 Mon 17:00 H21

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]Donostia 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 16.9 Mon 17:15 H21

Functional Renormalization Group Approach for Inhomogeneous One-Dimensional Fermi Systems with Finite-Ranged Interactions — •Lukas Weidinger, Florian Bauer, Jan Heyder, and Jan von Delft — LMU München, Arnold Sommerfeld Center for Theoretical Physics

We use the functional renormalization group (fRG) to study transport through quantum point contacts (QPCs) described by a one-dimensional lattice model with either on-site or finite-ranged interactions. In previous work on this model [Bauer2014], the so-called coupled-ladder approximation (CLA) was shown to admit a consistent fRG treatment for the case of a purely onsite interaction. We introduce an extended version of this scheme, called the extended coupled ladder approximation (eCLA), which includes a spatially extended feedback between the individual interaction channels, measured by a feedback length L. We applied a static version of this scheme to our QPC model, finding that for on-site interactions, this scheme converges to the third-order-truncated fRG when L is increased beyond the characteristic length l_x of the QPC. Additionally, it turns out that the enhanced feedback stabilizes the fRG flow. Furthermore, it allows us to also treat a finite-ranged interaction with a range of up to L sites. Studying our QPC model with a screened Coulomb interaction, we find that in certain parameter regimes (in particular interaction range $\gtrsim l_x$), the density shows the onset of crystaline features in the QPC region, accompanied by oscillatory behavior of the conductance as function of gate voltage.

TT 16.10 Mon 17:30 H21

Transport through strongly correlated Hubbard chains — •Junichi Ozaki and Yoshihiro Asai — AIST, Tsukuba, Japan

Strong correlation effect on the electric conductance of a wire at zero bias voltage was discussed a lot in the literatures mostly a decade ago by using the Luttinger model and/or some numerical methods. In some cases, the finite size effect of the single chain is not taken into account very well. Moreover, the effect of the thermalized Landauer*s electrode has not been taken into account quite unfortunately. Here, we put our priorities on these unresolved problems in discussing the strong correlation effect on the charge transport. The electric current in the strong correlation regime under the finite bias voltage is investigated in terms of a finite length single chain Hubbard model connected to non-interacting electrodes. The on-site Coulomb repulsion and the length are the variables. We use the time-dependent density matrix renormalization group (t-DMRG), which describes the many-body electron dynamics accurately. The zero-bias conductance and the current versus voltage (I-V) characteristics are examined at zero temperature. The conductance oscillation as a function of the length accompanies a damping. The non-linear behavior due to the strong correlation effect is found in the I-V curve. In the both cases, inelastic contribution from the Coulomb repulsion is clear in the strong correlation regime.

TT 17: Low-Dimensional Systems: Oxide Hetero-Interfaces

Time: Monday 15:00–17:15 Location: H22

TT 17.1 Mon 15:00 H22

Universal Fabrication of Two-Dimensional Electron Systems in Functional Oxides — •Tobias C. Rödel[1,2], Frank Fortuna[1], Shamashis Sengupta[3], Emmanouil Frantzeskakis[1], Patrick Le Fèvre[2], François Bertran[2], Bernard Mercy[4], Sylvia Matzen[5], Guillaume Agnus[5], Thomas Maroutian[5], Philippe Lecoeur[5], 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]Laboratoire de Physique des Solides, Univ. Paris-Sud, CNRS, Université Paris-Saclay, 91405 Orsay, France — [4]CRISMAT, ENSICAEN-CNRS UMR6508, 6 bd. Maréchal Juin, 14050 Caen, France — [5]Institut d'Electronique Fondamentale, Univ. Paris-Sud, CNRS, Université Paris-Saclay, 91405 Orsay, France

Two-dimensional electron systems (2DESs) in transition metal oxides are currently a field of intense research in the quest of novel functionalities in materials showing competing ground states. The 2DESs in $SrTiO_3$-based interfaces have been the cornerstone of such research. To go beyond, it is essential to create new types of oxide 2DESs in a technically easy way. Here we show, using (angle-resolved) photoemission spectroscopy in UHV that the deposition of atomically-thin layers of an elementary reducing agent results in the creation of 2DESs at the interface of several functional oxides, such as the ferroelectric $BaTiO_3$. This technique can be adapted for transport studies and opens the possibility to study 2DESs in strongly-correlated insulating oxides.

TT 17.2 Mon 15:15 H22

Gating effect in a lateral $LaAlO_3/SrTiO_3$ 2DEG - $SrTiO_3$ heterostructure — •Alexander Müller[1], Mohsin Minhas[1], Hans-Helmuth Blascheck[1], Bodo Fuhrmann[2], and Georg Schmidt[1,2] — [1]Fachbereich Physik, Martin-Luther Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

We have successfully patterned the two dimensional electron gas which forms at the interface between $LaAlO_3$ (LAO) and $SrTiO_3$(STO) [1] using electron beam lithography and reactive Ion Etching (RIE). With this process small gaps between electrodes were created which at low temperature show the characteristics of the channel of a tunneling field effect transistor. An additional side gate can be used to modulate the I/V characteristics and thus create a true three terminal device. At low temperatures the transistor exhibits a transconductance of 32 μA/V for a channel width of 4 μm and a sub threshold swing of 9 mV/dec.
[1] A. Ohtomo, H.Y. Hwang, Nature **427**, 6973 (2004)

TT 17.3 Mon 15:30 H22

Anisotropic transport in the two dimensional electron gas at oxide hetero-interfaces — •Roland Schäfer[1], Dirk Fuchs[1], Karsten Wolff[1,2], Ahmed Sleem[1,2], Richard Thelen[3], Rudolf Schneider[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe — [3]Karlsruher Institut für Technologie, Institut für Mikrostrukturtechnik, 76021 Karlsruhe

We observe a resistive transition to superconductivity in the two dimensional electron gas which forms at the interface of strontium titanate and lanthanum aluminate or amorphous aluminium oxide. Resistivity is measured on quadratic samples in van der Pauw geometry; the voltage drop resulting from current injected at two contacts on one side of the sample is probed at the opposite side by two further contacts. The two possible, orthogonal arrangements show distinct different behavior indicating strong anisotropy in the transport properties of the electron gas. The results will be discussed with respect to a reduced dimensionality of the superconducting condensate.

TT 17.4 Mon 15:45 H22

Non-Fermi-liquid behavior in δ-doped $SmTiO_3$ from first principles — •Frank Lechermann — I. Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg — Institut für Keramische Hochleistungswerkstoffe, Technische Universität Hamburg-Harburg, 21073 Hamburg

Most stoichiometric condensed matter underlying stronger electronic correlations comes in two flavors. Either the compound is metallic with usually well-defined quasiparticles at low energy, or it is in a Mott-(or charge-transfer-)insulating state with robust Hubbard bands at high energy seperated by a sizable charge gap. Doped Mott insulators are more difficult to characterize, since e.g. introduced itinerancy often has to cope with preexisting ordered states of magnetic kind. Furthemore, bulk doping of Mott insulators is plagued by disorder effects, which are hard to capture theoretically by simple means.

Novel oxide heterostructures provide an alternative way of doping Mott-insulating materials by introducing well-defined doping layers in given host materials. Recent experimental work on δ-doped titanates has shown the possibility for new emerging physics [1]. In this talk an advanced DFT+DMFT study of the δ-doped $3d^1$ titanate $SmTiO_3$ is presented. Layer- and temperature-dependent multi-orbital Mott transitions as well as spin and orbital polarizations are discussed. The intricate transport behavior in the conducting layers of the established itinerant interface state will be elucidated.
[1] C. A. Jackson, J. Y. Zhang, C. R. Freeze and S. Stemmer, Nat. Commun. **5**, 4258 (2014).

15 min. break

TT 17.5 Mon 16:15 H22

Magnetism, spin texture and in-gap states: Atomic specialization at the surface of oxygen-deficient $SrTiO_3$ — •Harald O. Jeschke[1], Michaela Altmeyer[1], Marcelo Rozenberg[2], Marc Gabay[2], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany — [2]Laboratoire de Physique des Solides, Bat 510, Université Paris-Sud, 91405 Orsay, France

We investigate the electronic structure and spin texture at the (001) surface of $SrTiO_3$ in the presence of oxygen vacancies by means of *ab initio* density functional theory (DFT) calculations of slabs. Relativistic non-magnetic DFT calculations exhibit Rashba-like spin winding with a characteristic energy scale $\sim$ 10 meV. However, when surface magnetism on the Ti ions is included, bands become spin-split with an energy difference $\sim$ 100 meV at the Γ point. This energy scale is comparable to the observations in SARPES experiments performed on the two-dimensional electronic states confined near the (001) surface of $SrTiO_3$. We find the spin polarized state to be the ground state of the system, and while magnetism tends to suppress the effects of the relativistic Rashba interaction, signatures of it are still clearly visible in terms of complex spin textures.

TT 17.6 Mon 16:30 H22

Pressure effects on the 2D electron system in $LaAlO_3/SrTiO_3$. — •Vladislav Borisov[1], Jone Zabaleta[2], Harald O. Jeschke[1], Thilo Kopp[3], and Roser Valenti[1] — [1]Institute of Theoretical Physics, Goethe University, D-60438 Frankfurt am Main, Germany — [2]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [3]Center for Electronic Correlations and Magnetism, Experimental Physics VI, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany

We present a theoretical study of pressure effects on the electronic properties of the $LaAlO_3/SrTiO_3$ (001) interface. Lattice relaxation plays a crucial role for the formation of the 2D electron system (2DES), in agreement with previous reports. We observe that the carrier density of the 2DES at zero pressure is much lower than the "polar catastrophe" estimate of 0.5 e^- per two-dimensional unit cell, which agrees with most experimental works. Under hydrostatic pressure, structural distortions in $LaAlO_3$ (LAO) are largely suppressed, whereas they increase in $SrTiO_3$ (STO), and the carrier density of the 2DES is enhanced by almost 45% using a moderate pressure of 4.1 GPa. The origin of this behavior as well as the explanation for the low carrier density at the interface at ambient pressure are discussed in terms of the lattice polarization and electronic Berry phase in the LAO oxide. Reduction of the calculated static dielectric constants of LAO and STO under pressure might account for the recent experimental findings [1] regarding the carrier mobility.
[1] J. Zabaleta et al. (in preparation).

TT 17.7 Mon 16:45 H22

Interplay of oxygen vacancies and electronic correlations in $SrVO_3$ — •Steffen Backes[1], Aaram J. Kim[1], Frank Lechermann[2], Harald O. Jeschke[1], Marcelo J. Rozenberg[3], Andres F. Santander Syro[4], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str.1, 60438 Frankfurt am Main, Germany — [2]Institut für Theoretische Physik, Universität Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany — [3]Laboratoire de Physique des Solides, Université Paris-Sud, Bâtiment 510, 91405 Orsay, France — [4]CSNSM, Université Paris-Sud and CNRS/IN2P3, Bâtiments 104 et 108, 91405 Orsay cedex, France

We investigate the role of oxygen vacancies in $SrVO_3$ within LDA+DMFT (density functional theory combined with dynamical mean-field theory). We show that, in addition to the usual t_{2g} lower Hubbard band, oxygen vacancies are responsible for an additional peak around -1 eV of V $3d_{z^2}$ orbital character, which is not present in the bulk system without vacancies. We discuss our results in the light of recent angle-resolved photoemission (ARPES) experiments.

TT 17.8 Mon 17:00 H22

Engineering the work function of oxide heterostructures — •Zhicheng Zhong and Philipp Hansmann — Max-Planck Institute for Solid State Research

The design of novel materials for new functionality that push the frontiers of technology is one of the most important challenges in electronic structure calculations. One specific technology, still in its infancy, presents an alternative to thermoelectric conversion of heat to electrical energy and was coined as the thermoelectronic approach. The key components of a thermoelectronic device are an electron emitter and an electron collector separated by a vacuum. The creation of an electron current in the vacuum and the efficiency of the device crucially depends on the absolute value and the ratio of the work functions of emitter and collector material. In our study we investigate work functions of various transition metal oxide surfaces and how we can tune the work function by manipulating the surface by heterostructuring.

TT 18: Spincaloric Transport (Joint session of MA and TT organized by MA)

Time: Monday 15:00–18:15 Location: H31

TT 18.1 Mon 15:00 H31

Spectral characteristics of time resolved magnonic spin Seebeck effect [1] — •levan chotorlishvili, seyyed etesami, and jamal berakdar — Institut für Physik, Martin Luther University Halle-Wittenberg, 06099 Halle/Saale, Germany

Spin Seebeck effect (SSE) refers to the generation of spin current due to a temperature gradient, in analogy to the conventional Seebek effect. The current work addresses and unvocer the role of subthermal magnons contributions to the SSE in insulating ferromagnets. The finding is in line with recent experiments given in Ref. [2], and points to further interesting experiments and material composition design aiming at enhancing/exploiting SSE. Technically, the spin-current dynamics is treated based on the Landau-Lifshitz-Gilbert (LLG) equation, while the formation of the time dependent thermal gradient being described self-consistently via the heat equation coupled to the magnetization dynamics. [3]

[1] S. R. Etesami, L. Chotorlishvili, and J. Berakdar, Appl. Phys. Lett. 107, 132402 (2015). [2] S. R. Boona and J. P. Heremans, Phys. Rev. B 90, 064421 (2014). [3] N. Roschewsky, M. Schreier, A. Kamra, F. Schade, K. Ganzhorn, S. Meyer, H. Huebl, S. Geprgs, R. Gross, and S. T. B. Goennenwein, Appl. Phys. Lett. 104, 202410 (2014).

TT 18.2 Mon 15:15 H31

A novel tool to investigate anisotropic effects in spin caloric measurements — •Oliver Reimer, Michel Bovender, Jan-Oliver Dreessen, Daniel Meier, Lars Helmich, Andreas Hütten, Jan-Michael Schmalhorst, Günter Reiss und Timo Kuschel — CSMD, Physics Department, Bielefeld University, Germany

In spin caloric measurements ∇T acts as a driving force for spin currents. A ferromagnet exposed to ∇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. In paramagnets the spin Nernst effect is expected to cause a transverse spin current which can induce a spin torque transfer at the interface to a magnetic material. Thus, ∇T could be used in combination with $\vec{H}$ to create a spin Nernst effect based magnetothermopower similar to the current driven spin Hall magnetoresistance [2,3]. We introduce a new setup which allows the rotation of ∇T in addition to varying T_{base} and ΔT. This talk gives an overview of the implementation of an infrared camera controlled rotation of ∇T which combined with the rotation of $\vec{H}$ enables the measurement of anisotropic spin caloric effects. The functionality of the setup is proven by planar Nernst effect measurements and compared to the results of D. Meier et al. [4].

[1] K. Uchida et al., Appl. Phys. Lett. 97, 172505 (2010)
[2] H. Nakayama et al., Phys. Rev. Lett. 110, 206601 (2013)
[3] M. Althammer et al., Phys. Rev. B 87, 224401 (2013)
[4] D. Meier et al., Phys. Rev. B 88, 184425 (2013)

TT 18.3 Mon 15:30 H31

Tunnel magneto-Seebeck effect in MgO tunnel junctions — •Ulrike Martens[1], Alexander Boehnke[2], Marvin von der Ehe[1], Christian Franz[3], Michael Czerner[3], Karsten Rott[2], Andy Thomas[2,4], Christian Heiliger[3], Günter Reiss[2], and Markus Münzenberg[1] — [1]Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, Germany — [2]CSMD, Physics Department, Bielefeld University, Germany — [3]Justus-Liebig-Universität Gießen, Germany — [4]IMW, IFW Dresden, Germany

In recent spincaloritronic research several groups have observed the tunnel magneto-Seebeck effect (TMS) in magnetic tunnel junctions (MTJs) incorporating CoFe electrodes and MgO tunnel barriers [1, 2]. Semiconducting materials are known to have large Seebeck coefficients. This is mainly attributed to the gap in their band structure and the asymmetric position of the Fermi-level. The tunnel magneto-Seebeck effect (TMS) is a powerful tool to investigate such spin-dependent Seebeck coefficients, because separate spin-channels can be defined in magnetic tunnel junctions (MTJs). Here, we investigate the spin-dependent Seebeck coefficients of CoFeB/MgO/CoFeB MTJs with different thicknesses of the MgO barrier. CoFeB/MgO/CoFeB MTJs with TMR ratios of 80% to 230% show TMS ratios of 5% to 50%. With a size variation of the heating laser spot we see zero crossing voltage compensation effects. Funding by DFG SPP 1538 is acknowledged.

[1] Walter, M., et al. Nature Mater. 10, 742 (2011)
[2] Liebing, N., et al. Phys. Rev. Lett. 107, 177201 (2011)
[3] A. Boehnke et al. Rev.Sci. Instrum 84 (2013)

TT 18.4 Mon 15:45 H31

Spincaloric properties of epitaxial $Co_2MnSi/MgO/Co_2MnSi$ magnetic tunnel junctions — •Benjamin Geisler[1,2] and Peter Kratzer[2] — [1]FRM II, Technische Universität München, 85748 Garching, Germany — [2]Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

Magnetic tunnel junctions (MTJs) with ferromagnetic, half-metallic electrodes are interesting spintronics devices due to their high tunnel magnetoresistance ratio. If a thermal gradient is applied to such a MTJ, the relative electrode magnetization can be detected by measuring the induced voltage, i.e., by exploiting the magneto-Seebeck effect.

Here we present an *ab initio* viewpoint on transport and spincaloric properties of epitaxial $Co_2MnSi/MgO(001)/Co_2MnSi$ MTJs [Phys. Rev. B 92, 144418 (2015)]. We compare results calculated with the conventional Sivan-Imry approach to results obtained from solving the Landauer-Büttiker equation directly. The latter procedure circumvents the linear response approximation inherent in the Seebeck coefficient and provides the response of the system (current or voltage) to arbitrary thermal gradients. Moreover, thermal variations of the chemical potential in the leads and finite-bias effects can be readily included in this method. Especially the former are found to be important here for obtaining qualitatively correct results. We show how the spincaloric properties of the MTJs depend on the interface atomic structure and that they can be tailored by a targeted growth control.

Finally, we shortly comment on the influence of thermally activated electrode phonons and interface magnons.

TT 18.5 Mon 16:00 H31

Current progress of the tunnel magneto-Seebeck effect in Heusler based MTJs — •Alexander Boehnke[1], Torsten Huebner[1], Ulrike Martens[2], Marvin von der Ehe[2], Christian Sterwerf[1], Christian Franz[3], Timo Kuschel[1], Andy Thomas[1,4], Christian Heiliger[3], Markus Münzenberg[2], and Günter Reiss[1] — [1]CSMD, Physics Department, Bielefeld University, Germany — [2]University of Greifswald, Germany — [3]University of Giessen, Germany — [4]IMW, IFW Dresden, Germany

The tunnel magneto-Seebeck effect (TMS) [1,2] describes the difference of the Seebeck coefficients S_p and S_{ap} of a magnetic tunnel junction (MTJ) in the parallel and antiparallel magnetization alignment. Obviously, increasing the difference between S_p and S_{ap} as well as their magnitude is desirable to reduce the signal-to-noise ratio, e.g. for determining the magnetic state of the MTJ in memory applications.

Here, we suggest MTJs with an MgO barrier and Heusler compound electrodes (e.g. Co_2FeAl, Co_2FeSi) as good candidates for fulfilling both goals, because of their half-metallic density of states [3]. We will present current results on TMS measurements performed on these MTJs and discuss how to optimize the choice of materials for future devices.

[1] Walter et al., Nature Mater. 10, 742 (2011).
[2] Boehnke et al. Rev. Sci. Instrum. 84, 063905 (2013).
[3] Geisler et al., Phys. Rev. B. 92, 144418 (2015).

TT 18.6 Mon 16:15 H31

Comparison of laser induced and intrinsic tunnel magneto-Seebeck effect in CoFeB/$MgAl_2O_4$/CoFeB magnetic tunnel junctions — •Torsten Huebner[1], Alexander Boehnke[1], Ulrike Martens[2], Markus Münzenberg[2], Andy Thomas[3], Timo Kuschel[1], and Günter Reiss[1] — [1]CSMD, Physics Department, Bielefeld University, Germany — [2]IFP, Greifswald University, Germany — [3]IMW, IFW Dresden, Germany

The Seebeck coefficient of a Magnetic Tunnel Junction (MTJ) depends on its magnetic state known as the tunnel magneto-Seebeck (TMS) effect [1]. It has been extensively studied with indirect Joule and laser induced heating [2,3]. Zhang, Teixeira et al. [4,5] proposed a third method using the intrinsic Joule heating by the tunneling current without any external temperature gradient. Here, we prepared CoFeB/$MgAl_2O_4$/CoFeB MTJs and obtained a maximum tunnel magneto-resistance (TMR) ratio of 34 % at room temperature for a nominal barrier thickness of 1.8 nm. We used a modulated diode laser (P_{max}=150 mW, λ=637 nm, f=177 Hz) to generate a temperature gradient across the junctions and recorded IU-characteristics to compare the laser induced TMS with the intrinsic TMS.

15 min. break

TT 18.7 Mon 16:45 H31

Influence of laser heating on switching fields in magnetic tunnel junctions — •Hangfu Yang, Niklas Liebing, Xiukun Hu, Sibylle Sievers, Mark Bieler, and Hans W. Schumacher — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

The field of spin caloritronics focuses on the interplay between heat, charge and spin currents in magnetic systems and gained a lot of interest due to new phenomena such as the tunnel magneto-Seebeck effect [1] and the thermal spin transfer torque [2]. Here, we study the influence of temperature and temperature gradients on magnetic switching of the free layer of CoFeB/MgO/CoFeB magnetic tunnel junctions (MTJs). Thermal gradients across the MTJs are generated locally by femtosecond laser pulses. The switching of the free layer is determined by magnetostatic measurements of the critical switching curve as a function of the laser power. We find that the entire critical curve shifts up to 4 mT along the easy axis at a laser power of 110 mW. We show that the shift in the critical curve is caused by an increase of the overall temperature due to heat accumulation rather than by a temperature gradient. Future studies will focus on reducing the stationary temperature increase, allowing for the generation of larger temperature gradients in our samples.

[1] N. Liebing et al., Phys. Rev. Lett. 107, 177201 (2011); M. Walter et al., Nature Mater. 10, 742-746 (2011).
[2] M. Hatami et al., Phys. Rev. Lett. 99, 066603 (2007); G.M. Choi et al., Nature Phys. 11, 576-581 (2015).

TT 18.8 Mon 17:00 H31

Thickness-dependent low-temperature enhancement of the spin Seebeck effect in YIG films — •Joel Cramer[1], Er-Jia Guo[1,2], Andreas Kehlberger[1], Christoph Schneider[1], Gerhard Jakob[1], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]Quantum Condensed Materials Division, Oak Ridge National Laboratory, TN 37830, Oak Ridge, USA

In ferromagnetic insulator (FMI)/normal metal (NM) bilayers the temperature dependence of the spin Seebeck effect (SSE) has been probed as a function of FMI thickness, different interfaces and detection materials [1, 2]. At low temperatures, an enhancement of the SSE signal is observed, including the appearance of a peak in the amplitude. This enhancement is more pronounced for thicker films and vanishes for film thicknesses below 600 nm. Furthermore, the temperature of the signal maximum strongly depends on the FMI thickness as well as on the FMI/NM interface. The thickness dependence can be well explained by considering a model of a magnon-driven SSE, which takes into account the frequency dependent propagation length of thermally excited magnons inside the bulk material. The NM dependence, however, indicates that previously neglected interface effects play a major role in the observed signal. In order to obtain a better understanding of the influence of the FMI/NM interface, transmission electron microscopy (TEM) measurements combined with elemental analysis (EELS) are performed. [1] A. Kehlberger et al. Phys. Rev. Lett. 115, 096602 (2015) [2] Er-Jia Guo et al. arXiv: 1506.06037

TT 18.9 Mon 17:15 H31

Static magnetic proximity effect in Pt layers on sputter deposited $NiFe_2O_4$ and on Fe of various thicknesses investigated by x-ray resonant magnetic reflectivity — •Panagiota Bougiatioti[1], Christoph Klewe[1], Olga Kuschel[2], Joachim Wollschläger[2], Laurence Bouchenoire[3,4], Simon D. Brown[3,4], Jan-Michael Schmalhorst[1], Daniel Meier[1], Günter Reiss[1], and Timo Kuschel[1] — [1]CSMD, Physics Department, Bielefeld University, Germany — [2]Fachbereich Physik, Universität Osnabrück, Germany — [3]XMaS, ESRF, Grenoble, France — [4]University of Liverpool, UK

In this project we implemented x-ray resonant magnetic reflectivity (XRMR) to investigate magnetic proximity effects (MPE) in Pt films on sputter deposited $NiFe_2O_4$(260 nm) (NFO) and in Pt/Fe(x nm) samples with x from 1.1 nm to 18.2 nm. We did not observe a magnetic response down to a limit of 0.04 μ_B per Pt atom regarding the sputter deposited NFO bilayer, in agreement to previously investigated chemical vapor deposited NFO samples [1]. We performed longitudinal spin Seebeck effect measurements on this bilayer system and exclude an anomalous Nernst effect induced by the MPE in Pt down to a certain limit. Furthermore, we confirm the independence of the MPE from the thickness of the magnetic layer (Fe), unveiling its sensitivity to the interface properties of the magnetic material [2].

[1] T. Kuschel et al., Phys. Rev. Lett. 115, 097401 (2015)
[2] T. Kuschel et al., submitted to IEEE Trans. Magn. (2015)

TT 18.10 Mon 17:30 H31

Temperature dependence of the domain wall magneto-Seebeck effect — •Alexander Fernández Scarioni, Patryk Krzysteczko, Xiukun Hu, Niklas Liebing, Sibylle Sievers, and Hans W. Schumacher — Physikalisch-Technische Bundesanstalt, Bundesallee 100, D-38116, Braunschweig, Germany

We study the thermopower response of a magnetic domain wall in a nanowire under the influence of a thermal gradient and compare it with corresponding magnetoresistance measurements. The nanowire used is an L-shape permalloy (Ni80Fe20) nanowire. A single domain wall can be nucleated and pinned at a notch between two electrical contacts. We observe a clear thermopower signature of the domain wall pinned at the notch.

The thermal gradient is generated by an electrical microheater placed in the vicinity of the magnetic nanowire. We study the local heat distribution experimentally by microscopic resistance thermometers and numerically by finite element calculations.

By combination of thermal gradient and magnetothermopower measurements at various temperatures we can describe the system based on the anisotropic magneto-Seebeck effect.

TT 18.11 Mon 17:45 H31

Thermally excited magnon accumulation in complex magnetic materials — •Ulrike Ritzmann, Denise Hinzke, and Ulrich Nowak — Universität Konstanz, Konstanz, Germany

It was shown experimentally that in a magnetic insulator spin currents can be created by applying temperature gradients [1]. Using atomistic spin model simulations, we study magnonic spin currents and their characteristic length scales in ferromagnetic materials with different temperature profiles [2,3,4]. Furthermore, we explore thermally excited spin currents in antiferromagnetic materials and study the magnon accumulation in the vicinity of a temperature step and its characteristic length scale. We determine the different antiferromagnetic modes that are excited and discuss their propagation length using an one-dimensional analytical model.

These methods can be extended for ferrimagnetic materials. In a two-sublattice ferrimagnet, we determine the thermally excited magnon accumulation due to a temperature step. We study the temperature dependence of the magnon accumulation in ferrimagnets and investigate under which condition the magnon accumulation in such systems vanishes.

We acknowledge financial support by the DFG through SFB 767 and through SPP "Spin Caloric Transport".

[1] K. Uchida et al, Appl. Phys. Lett. **97**, 172505 (2010)
[2] U. Ritzmann et al., Phys. Rev. B **89**, 024409 (2014)
[3] A. Kehlberger et al.,Phys. Rev. Lett. **115**, 096602 (2015)
[4] U. Ritzmann et al., Phys. Rev. B **92**, 174411(2015)

TT 18.12 Mon 18:00 H31

Spin wave scattering and localization effects due to defects in magnetic materials — •Martin Evers, Cord A. Müller, and Ulrich Nowak — University of Konstanz, 78457 Konstanz, Germany

From earlier studies of transport of particles and waves it is known that there are different transport regimes. E.g. in a perfect crystal transport will be ballistic, but one usually has to deal with some kind of imperfections that induce disorder in the system. As Anderson has shown in 1958 in case of phase coherent transport disorder can also lead to completely suppressed transport, known as Anderson localization [1]. For the case of spin waves this will lead to a vanishing magnon propagation length, even without any damping mechanism [2,3].

Within a classical spin model utilizing the Landau-Lifshitz-Gilbert equation we study coherent backscattering (CBS), which is a weak localization phenomena and therefore a precursor for Anderson localization, in 2D. Especially the influence of non-linearities, damping and the Dzyaloshinskii-Moriya interaction is investigated. We also find evidence for coherent forward scattering [4] of magnons in a quasi one-dimensional setting, providing a direct signal of Anderson localization and absence of thermalization.

[1] P. W. Anderson, Phys. Rev. **109**, 1492 (1958)
[2] U. Ritzmann et al., Phys. Rev. B **89**, 024409 (2014)
[3] M. Evers et al., Phys. Rev. B **92**, 014411 (2015)
[4] T. Micklitz et al., Phys. Rev. Lett. **112**, 110602 (2014)

TT 19: Superconductivity: Poster Session

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

TT 19.1 Mon 15:00 Poster D

Superconductivity in the high-pressure phase of bismuth — •Philip A. C. Brown, Konstantin Semeniuk, and F. Malte Grosche — Department of Physics, Cavendish Laboratory, University of Cambridge, UK

At pressures above 27 kbar, elemental bismuth adopts a highly unusual incommensurate host-guest structure. This structure combines two distinct, interpenetrating crystal lattices and consequently lacks discrete translational symmetry. Although similar high pressure structures have been observed in other elements, their electronic properties have not been investigated in detail. The moderate pressure required to induce the host-guest phase in bismuth presents a favourable opportunity for comprehensive electrical transport studies.

The high-pressure host-guest phase of bismuth, termed Bi-III, is known to be superconducting with a transition temperature of around 7 K, but the details of its superconducting and normal state properties are comparatively little explored. We report resistivity and magnetisation measurements in the Bi-III phase in fields up to 9 T and temperatures down to 120 mK. We find evidence for a strikingly high critical field and an unusual temperature dependence of the resistivity above the superconducting transition. We discuss our findings in the context of theoretical descriptions of host-guest materials.

TT 19.2 Mon 15:00 Poster D

Co-sputtered MoRe as carbon nanotube growth-compatible superconductor — •Karl Götz, Stefan Blien, Peter Stiller, Ondrej Vavra, Thomas Mayer, Thomas Huber, Thomas Meier, Matthias Kronseder, Christoph Strunk, and Andreas Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Molybdenum rhenium alloys exhibit superconducting transition temperatures up to 15 K as well as high critical current densities. In addition, the thin films are stable under typical carbon nanotube CVD growth conditions, i.e., a hydrogen/methane atmosphere at 900 °C, and form good contacts in nanotube overgrowth. This makes them predestined for experiments integrating "ultraclean" carbon nanotube devices into coplanar radiofrequency circuits, towards quantum nanoelectromechanics and information processing. MoRe thin films are deposited via co-sputtering of two separate targets. The resulting thin film composition and its controllability is verified via XPS spectroscopy both before and after undergoing nanotube growth conditions. The effects of the high temperature process on surface oxides, carbon content, superconducting critical temperature, magnetic field, and current are characterized. Selecting an optimized alloy composition, we define coplanar waveguide resonators, demonstrating resonant behaviour after CVD at $f \approx 3 \ldots 4$ GHz and up to $Q_\mathrm{i} \approx 5000$. Modelling device properties via Mattis-Bardeen theory combined with substrate two-level systems leads to good agreement with the data.

TT 19.3 Mon 15:00 Poster D

Magnetic field dependent microwave spectroscopy on superconducting Pb stripline resonators — •Nikolaj G. Ebensperger, Markus Thiemann, Martin Dressel, and Marc Scheffler — 1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, D-70569 Stuttgart, Germany

Planar superconducting resonators have multiple applications, e.g. in quantum information processing or spectroscopy on unconventional solids. Here, Pb can be used as a basis of microwave resonators with a critical temperature of 7.2 K and a critical magnetic field of 80 mT. It shows interesting behavior with residual normal conducting areas after entering the superconducting phase with applied external magnetic field.

We present a study of superconducting Pb microwave stripline resonators in variable external magnetic field up to 140 mT and a temperature range of 1.6 K to 6.5 K. We are able to determine the complex conductivity of Pb in variable magnetic field and we find striking similarities to measurements in variable temperature, like a coherence peak. The quality factor of the resonances shows strong hysteresis effects after exceeding the critical magnetic field, indicating residual normal conducting areas in the resonator persisting in the superconducting state. We are able to determine the critical magnetic field for a set of given temperatures both for the Pb resonator as well as a Sn sample placed on top of the underlying Pb resonator. These results demonstrate that Pb resonators can be applied for different spectroscopy studies in zero as well as finite magnetic field.

TT 19.4 Mon 15:00 Poster D

Microwave study of superconducting Sn films above and below percolation — •Manfred H. Beutel, Nikolaj G. Ebensperger, Markus Thiemann, Gabriele Untereiner, Martin Dressel, and Marc Scheffler — 1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, D-70569, Germany

The electronic properties of superconducting Sn films ($T_c \approx 3.7$ K) change significantly when lowering the film thickness down to a few nm, in particular at the percolation threshold. The low energy electrodynamics of such Sn samples can be probed via microwave spectroscopy,

e.g. with superconducting stripline resonators.

We have deposited Sn films by thermal evaporation, ranging in thickness between 38 nm and 842 nm, and we characterized their morphology by AFM. We use superconducting Pb stripline resonators to probe the microwave response of Sn films at temperatures from 7.5 K down to 1.5 K in a frequency range between 1 GHz and 20 GHz. The measured quality factor of the resonators decreases with increasing temperature due to increasing losses. As a function of the sample thickness we observe three regimes with significantly different properties: Samples below percolation exhibit dielectric properties with negligible losses, demonstrating that macroscopic current paths are required for appreciable dynamical conductivity of Sn at GHz frequencies. Thick Sn films, on the other hand, lead to low-loss resonances above and below T_c of Sn, but in an intermediate thickness regime, just above percolation, the metallic state of the Sn films is too lossy for resonator operation whereas the superconducting state only has low microwave losses.

TT 19.5 Mon 15:00 Poster D

Superconducting coplanar resonators with frequencies up to 50 GHz — •Markus Thiemann[1], Desirée Rausch[1], Martin Dressel[1], Daniel Bothner[2], Reinhold Kleiner[2], Dieter Koelle[2], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Physikalisches Institut and Center for Quantum Science in LISA$^+$,Universität Tübingen

Planar superconducting microwave resonators are widely used, e.g. in the field of quantum information technology, but usually at frequencies well below 20 GHz. Because of their high quality factor and therefore high sensitivity, superconducting planar resonators are very interesting probes for investigating the electronic properties of novel superconductors. The energy gap of superconductors with a $T_c < 1$ K lies within the GHz-regime. Hence, resonators covering a wide frequency range are desirable to perform measurements across the superconducting energy gap.

Therefore we have developed coplanar resonators, made of superconducting niobium ($T_c \approx 9.2$ K) on sapphire with operating frequencies up to 50 GHz. We show measurements performed on two different resonator designs with fundamental resonance frequencies of 2 GHz and 5 GHz, at ^{4}He temperatures. By measuring not only the fundamental mode, but also the higher harmonics, frequencies up to 50 GHz can be covered, showing quality factors exceeding 20000. To demonstrate the applicability of these resonators for spectroscopic measurements, we show measurements performed on bulk tin ($T_c \approx 3.7$ K), where the superconducting transition of tin can be observed up to 50 GHz.

TT 19.6 Mon 15:00 Poster D

Measuring the microwave response of superconducting Nb:STO and Ti at mK temperatures using superconducting resonators — •Markus Thiemann[1], Manfred Beutel[1], Martin Dressel[1], Evangelos Fillis-Tsirakis[2], Hans Boschker[2], Jochen Mannhart[2], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Max Planck Institute for Solid State Research, Stuttgart

Niobium doped $SrTiO_3$ is a superconductor, with 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 $T_c \approx 0.3$ K . The superconducting dome may originate from the different bands being occupied depending on the doping level. The low energy scales of the system, as indicated by the low T_c are within the GHz-regime. Therefore microwave measurements are a powerful technique to reveal the electronic properties of these superconductors.

We preformed microwave measurements on Nb:STO of different doping levels in a dilution refrigerator, using superconducting stripline resonators. Measurements were done in a temperature and frequency range from 40-400mK and 1-20GHz, covering the normal and superconducting states. For comparison we also measured the temperature dependence of the surface impedance of superconducting titanium ($T_c \approx 0.5$ K), which can be well described by the Mattis-Bardeen equations with a ratio $\frac{2\Delta}{k_B T_c} = 3.56$. Therefore titanium is an ideal reference sample representing a conventional BCS-superconductor.

TT 19.7 Mon 15:00 Poster D

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

We have measured the conductance of square shaped TiN films on the superconducting and the insulating side of the superconductor/insulator transition. The conductance shows thermally activated behaviour with an activation energy $k_B T_0(L) \propto \ln L$, with L being the lateral size of the squares. Such behavior is consistent with 2D long-ranged Coulomb interactions with a large electrostatic screening length $\Lambda \simeq 200\,\mu$m [1]. To independently test whether long ranged Coulomb interactions can be responsible for the observed size dependence we compare $R(T, B)$ of a large TiN film in the critical region with and without a screening Pd layer in a distance $t \approx 60$ nm to the TiN film. The screening Pd-layer is expected to reduce the activation energy from $\propto \ln[\min(L, \Lambda)]$ to $\propto \ln(t)$ and the thermally activated resistance in films with $L \gtrsim \Lambda$ by the large number $\Lambda/t \simeq 3000$. In contrast, our experiment showed no significant reduction of $R(T)$ and T_0. This suggests that the measured size dependent conductance of our TiN film is not related to long-ranged Coulomb interactions.

[1] M. V. Fistul, V. M. Vinokur, and T. I. Baturina, PRL **100**, 086805 (2008).

TT 19.8 Mon 15:00 Poster D

The Polar Kerr Effect in Superconductors — •Joshua Robbins, James F. Annett, and Martin Gradhand — University of Bristol, United Kingdom

The polar Kerr effect is an optical phenomenon which arises in states with broken time-reversal symmetry. This effect has recently been observed in a series of unconventional superconductors, including the layered perovskite compound Sr_2RuO_4[1]. Confirmation of a Kerr signal below T_c supports the hypothesis of chiral p-wave superconductivity in this material. However, the nature of the unconventional superconducting state remains a source of controversy.

Here, we present calculations for the chiral superconducting state including spin-orbit coupling (SOC) by extending the three dimensional, multiband model considered previously [2]. SOC was found to induce strong mixing of the orbital characters within the bandstructure. This mixing is essential for the existence of the polar Kerr effect and the large increase due to SOC has a significant influence on the frequency dependence of the predicted Kerr signal.

We will extend and apply the model to other unconventional superconductors which have displayed the Kerr effect in recent years [3]. This will allow a detailed study of the symmetry properties of these systems and will provide valuable insight into the pairing mechanism of superconductors.

[1] J. Xia *et al.*, PRL **97**, 167002 (2006)
[2] M. Gradhand *et al.*, PRB., **88**, 094504 (2013)
[3] A. Kapitulnik *et al.*, NJP **11**, 055060 (2009)

TT 19.9 Mon 15:00 Poster D

Spin susceptibility and magnetic instability in Spin-Orbit Coupled system of Sr_2RuO_4 — Sergio Cobo[1], Ilya Eremin[2], and •Alireza Akbari[1] — [1]Asia Pacific Center for Theoretical Physics, Pohang, Gyeongbuk 790-784, Korea — [2]Theoretische Physik III, Ruhr-Universität Bochum - D-44780, Bochum, Germany

Although the Stronthium Ruthenate compound has been known for more than two decades, there are some major features, which still remain unknown. Mainly, it is still not clear what is the Cooper pairing mechanism and why it can be a triplet superconductor. These features turn out to be even more striking when considering the similarity of its crystal structure and that of the high-T_c cuprates. We analyzed the magnetic response of Sr_2RuO_4 under the presence of a strong spin-orbit coupling interaction. We found very remarkable anisotropies in the different components of the spin susceptibility. This finding strongly suggest that the Cooper instability may be driven by magnetic fluctuations and that spin orbit coupling is much more important than expected in this regard. Furthermore, we think there must be a relation between this interesting behavior and the fact that the stronthium ruthenate chooses the triplet-pairing channel when reaching the superconducting state.

TT 19.10 Mon 15:00 Poster D

Quasiparticle interference in heavy fermion superconductors: role of the slab geometry — •Fabian Lambert[1], Alireza Akbari[3,4], Peter Thalmeier[5], and Ilya Eremin[1,2] — [1]Institute für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Institute of Physics, Kazan (Volga Region) Federal University, 420008 Kazan, Russian Federation — [3]Asia Pacific Center for Theoretical Physics (APCTP) — [4]Department of Physics, and Max

Planck POSTECH Center for Complex Phase Materials, POSTECH, Pohang 790-784, Korea — [5]Max Planck Institute for the Chemical Physics of Solids, D-01187 Dresden, Germany

We analyze theoretically the quasiparticle interference in the heavy fermion superconductors $CeCoIn_5$ and UPt_3 as a direct method to investigate the gap symmetry. In contrast to the prior attempts that computed QPI patterns for some effective two-dimensional models or by perfoming calculations for varous k_z cuts and then averaging the final result, we perfom the calculations for the three-dimensional models in the slab geometry and investigate possible effects of the finite sample size, topology, and surface termination. Comparing with the results of prior analysis of the bulk system we can conclude on the importance of the possible surface states for determining the QPI pattern.

TT 19.11 Mon 15:00 Poster D

Magnetic properties of $La_{2-x}Sr_xCuO_4$: LDA+(C)DMFT study — •Amin Kiani and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

High temperature superconductivity in hole-doped cuprates is one of the most intriguing phenomena discovered in strongly correlated materials. In the normal phase, hole-doping causes the gradual destruction of antiferromagnetism and, in some cases, the appearance of incommensurate magnetic instabilities. In this work we study the magnetic properties of one of the representative family of materials, $La_{2-x}Sr_xCuO_4$. We calculate the static lattice spin susceptibility $\chi(\mathbf{q}, T)$ by using the local density approximations+dynamical mean field theory (LDA+DMFT) approach and the local vertex approximation. We discuss the results as a function of doping in the interval $0 \leq x \leq 0.4$ and investigate the non-local effects on $\chi(\mathbf{q}, T)$ via the cellular DMFT (CDMFT) approach.

TT 19.12 Mon 15:00 Poster D

Overgrowth of cracks in $YBa_2Cu_3O_{6+\delta}$-thin films grown on $SrTiO_3$- and Al_2O_3-substrates — •Kai Ackermann, Jens Hänisch, and Bernhard Holzapfel — Institut für Technische Physik, Karlsruher Institut für Technologie, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

High temperature superconducting materials like REBCO-thin films offer a wide range of applications like superconducting transformers, cables, coils or fault current limiters. Although the number of applications is increasing the REBCO-coated conductor length is still limited due to substrate and thin film fabrication defects. In order to improve the manufacturing processes of REBCO-coated conductors the growth behavior of REBCO-thin films on defective or broken substrate surfaces has to be understood. Therefore we investigated the structural and electronic properties of YBCO-thin films grown on cracked $SrTiO_3$- and Al_2O_3-substrates. The YBCO-films were prepared by using metalorganic (MOD) and pulsed laser deposition (PLD). Structural and electronic properties of the YBCO-films were investigated by using x-ray diffractometry, atomic force microscopy, scanning electron microscopy and temperature- and magnetic field-dependent conductivity measurements.

TT 19.13 Mon 15:00 Poster D

Measurements of the magnetic vortex lattice in the noncentrosymmetric superconductor Ru_7B_3 — •Yuliia Tymoshenko[1], Alistair Cameron[1], Geetha Balakrishnan[2], Monica Ciomaga Hatnean[2], Don McK. Paul[2], and Dmytro Inosov[1] — [1]Institut für Festkörperphysik, TU Dresden, D-01069 Dresden, Germany — [2]Department of Physics, University of Warwick, Coventry, CV47AL, United Kingdom

The noncentrosymmetric (NCS) superconductor Ru_7B_3 has a hexagonal structure within the [001] plane. NCS superconductors are of significant interest to the condensed matter community, as their crystal structure breaks inversion symmetry, leading to novel superconducting states with unusual properties. Such states associated with NCS superconductors have been predicted to have a significant effect on the vortex lattice (VL) within these materials. We investigated a large single crystal of Ru_7B_3 by small-angle neutron scattering (SANS). Our goal was to explore the possible influence of the NCS crystal structure on the VL order. During our measurements at the D33 SANS diffractometer at the Laue-Langevin Institute (ILL) in Grenoble, France we clearly observed the formation of VL in Ru_7B_3. The VL maintains its orientation and remains isotropic within the whole studied field and temperature range, implying a similar degree of isotropy in the SC parameters. An unusual VL rotation with decreasing field at base temperature was seen for field parallel to the (100) direction.

TT 19.14 Mon 15:00 Poster D

Interplay of SDW and iCDW order in iron-based superconductors: role of spin-orbit coupling — •Felix Ahn, Felix Lochner, and Ilya Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44801 Bochum, Germany

We study the interplay of SDW and iCDW order in iron-based superconductors and find that both orders couple to each other due to spin-orbit coupling. Most importantly, we analyze the influence of the CDW formation on the competition between various magnetic phases in iron-based superconductors.

TT 19.15 Mon 15:00 Poster D

Superfluid density and superconducting transition temperature in dirty iron-based superconductors — •Thomas Hartmann, Felix Ahn, and Ilya Eremin — Ruhr-Universität Bochum, Bochum, Deutschland

Measurements on optimally electron doped $LaFeAsO_{1-x}F_x$ samples under pressure up to $\sim$ 23 kbar reveal a clear mutual independence between the critical temperature T_c and the ratio of superfluid density over effective band mass of Cooper pairs n_s/m^*. The ratio increases about $\sim$ 30% at the maximum pressure whereas T_c remains constant, which clearly implies a breakdown of the Uemura relation in $LaFeAsO_{1-x}F_x$ [1]. Here we analyze theoretically this effect by taking into account the effect of nonmagnetic impurities in a multiband superconductor. We show that the ratio between intra-band and inter-band scattering rates can explain the behaviour of the observables under pressure by only acting on structural parameters while the amount of chemical disorder is still constant.
[1] G. Prando *et al.*, PRL **114**, 247004 (2015)

TT 19.16 Mon 15:00 Poster D

Spin response in LiFeAs and NaFeAs iron-pnictides superconductors — •Felix Lochner, Felix Ahn, and Ilya Eremin — Ruhr-Universität Bochum, Bochum, Deutschland

We analyze the spin susceptibility in LiFeAs and NaFeAs by using the ten-orbital tight-binding model that we fitted to the electronic band structure measured by recent ARPES experiments. We identify an effective five-band model for a weak k_z-dependence. Besides we present the bare and RPA-susceptibility and its q_z dependencies to study the magnetic instabilities and estimate the strength of intra-orbital and inter-orbital nesting.

TT 19.17 Mon 15:00 Poster D

Electronic correlations in the superconductors $A\mathbf{Fe_2As_2}$ with A = K, Rb, and Cs — •Sebastian Kuntz[1], Felix Eilers[1], Kai Grube[1], Diego A. Zocco[1], Peter Schweiss[1], Rolf Heid[1], Thomas Wolf[1], Peter Adelmann[1], and Hilbert von Löhneysen[1,2] — [1]Karlsruhe Institute of Technology, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruhe Institute of Technology, Physikalisches Institut, 76131 Karlsruhe, Germany

The stoichiometric iron-pnictide superconductors AFe_2As_2 exhibit a diverging effective mass of the normal-conducting quasiparticles with increasing alkali-metal ion radius R_A. This divergence suggests the proximity to a quantum phase transition (QPT) at negative pressures. We have performed thermal expansion, magnetostriction and magnetization measurements to characterize the normal and superconducting properties. We determined the phase diagrams as a function of the magnetic field parallel and perpendicular to the c axis. The measurements reveal the presence of several bands. The quasi-two-dimensional electronic structure of these layered materials leads to a Pauli limitation of the superconductivity for fields perpendicular to the c axis. The influence of the nearby QPT will be discussed and compared with the behavior of other related Fe-based superconductors.

TT 19.18 Mon 15:00 Poster D

Crystal growth and characterization of $SrFe_2(As_{1-x}P_x)_2$ — •Fryni Baglatzi, Agnes Adamski, and Cornelius Krellner — Physikalisches Institut, Goethe Universität Frankfurt am Main, D-60438, Frankfurt am Main

The discovery of iron-based superconductors brought new excitement to the field of unconventional superconducting (SC). Most studied are the so called (122 compounds), the AFe_2As_2 with A=Ba, Sr or Ca . An important point is, that different substitution series reveal different temperature-concentration phase diagrams, including varying SC

order parameters and coexistence regions of magnetism and SC.

The crystal growth of $SrFe_2As_2$ can be achieved by using the self-flux technique. However, exact melting temperatures of various flux to composition ratios are not reported in literature. We determined the melting points for various flux concentrations, using differential thermal analysis (DTA) in order to find out the pseudo binary phase diagram. Furthermore, crystal growth was conducted on the phosphorous doped series. Our samples were analyzed with scanning electron microscope, energy dispersive x-ray analysis and powder diffractometry, in order to determine the phase relations and distribution coefficients.

TT 19.19 Mon 15:00 Poster D

Magnetism and Superconductivity in $LaFeP_{1-x}As_xO$ — •Sirko Kamusella[1], Rajib Sarkar[1], Hubertus Luetkens[2], Setsuko Tajima[3], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [3]Department of Physics, Osaka University, Osaka 560-0043, Japan

The $LaFeP_{1-x}As_xO$ series bridges the gap between two parent compounds, whose Fermi surfaces differ in dimensionality and position of hole pockets. The resulting phase diagram consists of a superconducting two-dome structure separated by a novel AFM2 magnetic phase [1,2]. Electron doping by (O,F) substitution allows to investigate superconductivity in the full x-range.

^{57}Fe Mössbauer spectroscopy successfully depicts the temperature dependence of the tiny 0.1 μ_B magnetic moment in the AFM2 phase and its rigidity in applied field; with the help of a line width reference absorber. This uncommon approach makes Mössbauer measurements competitive to other local probe methods such as NMR or μSR.

μSR measurements can prove the long range character of this novel AFM2 phase and show the continuous change from a nodal to a nodeless symmetry of the superconducting order parameter upon substitution of P by As. AFM spin fluctuations suggested by NMR before [2] did not become evident in μSR decoupling experiments.

[1] K.T. Lai *et al.*, PR **90**, 064504 (2014)
[2] S. Miyasaka *et al.*, J. Phys. Soc. Jpn. **82**, 124706 (2013)

TT 19.20 Mon 15:00 Poster D

Scanning tunneling microscopy on bulk FeSe — •Jonas Dressner, Jasmin Jandke, Thomas Wolf, and Wulf Wulfhekel — Karlsruhe Institut of Technology, Germany

We used high-resolution scanning tunneling spectroscopy to study bulk FeSe at temperatures down to 30 mK. At this temperature, highly resolved spectra of the quasiparticle density of states could be measured showing multiple superconducting gaps. This is in agreement with the multiband character of this system. Furthermore, features of bosonic excitations are observed in the measured quasiparticle density of states and will be discussed.

TT 19.21 Mon 15:00 Poster D

Epitaxial growth of Fe-based superconductor thin films — Sven Meyer, •Jens Hänisch, and Bernhard Holzapfel — Institut für Technische Physik, Karlsruher Institut für Technologie, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

The Fe-based superconductors (FBS), discovered in 2008, are not only interesting for possible applications due to their large upper critical fields and low anisotropies, but also for basic understanding of unconventional superconductivity. With their properties, they constitute a link between the classic low-T_c superconductors (low anisotropies, low thermal fluctuations, s-wave type symmetry) and the oxocuprates (T_c up to 55 K, large H_{c2}, unconventional pairing). Their multi-band nature reminds of MgB_2. We prepare thin films of FBS in the so called 122 family, namely Co- and P-doped $BaFe_2As_2$ to investigate application relevant properties, such as critical current density J_c, by pulsed laser deposition using a frequency-tripled Nd:YAG laser (λ = 355 nm). Microstructure and chemical composition will be investigated by XRD, AFM and SEM, and electrical transport using a 14 T PPMS. The results are compared to literature data on films grown at different wavelengths [1].

[1] H. Hiramatsu et al., APL **104**, 172602 (2014)

TT 19.22 Mon 15:00 Poster D

Physical Properties of Off-Stoichiometric LiFeAs — •Uwe Gräfe[1], Shiv Jee Singh[1], Robert Beck[1], Hans-Joachim Grafe[1], Sabine Wurmehl[1,3], Christian Hess[1,2], and Bernd Büchner[1,3] — [1]IFW Dresden, Institut für Festkörperforschung, Postfach 270116 01171 Dresden — [2]Center for Transport and Devices, TU Dresden, 01169 Dresden — [3]Institut für Festkörperphysik, TU Dresden, 01062 Dresden

It is known that small modifications on the stoichiometry of LiFeAs have high impact on the physical properties in the normal and superconducting state. Here we present a systematic study on the Li-Fe-As system by XRD, NQR and resistivity. We synthesized samples with different nominal compositions of Li, Fe and As by solid state reaction and show that, besides stoichiometric LiFeAs, only enriching the system with Fe forms phase pure samples. The modifications due to this enrichment can be tracked by a shift of the NQR-frequency and the lattice constants. Thus NQR can be taken as a measure for the changes induced by additional Fe in Li-Fe-As. We further show that these changes are not only decreasing T_c but also cause a sudden reduction of normal state resistivity and electron-electron scattering. Altogether we therefore conclude that Fe has a charge doping effect on Li-Fe-As.

TT 19.23 Mon 15:00 Poster D

Dynamic properties of $Ca_{10}(Pt_3As_8)(Fe_{1-x}Pt_xAs)_{10}$ in the superconducting state explored by NMR in high fields — •Felix Brückner[1], Rajib Sarkar[1], Arneil P. Reyes[2], Philip L. Kuhns[2], Maksym Surmach[1], Dmytro Inosov[1], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, TU Dresden, Dresden, Germany — [2]National High Magnetic Field Laboratory, Tallahassee, Florida, USA

The triclinic iron-based superconductor $Ca_{10}(Pt_3As_8)(Fe_{1-x}Pt_xAs)_{10}$ with a T_c of 13 K exhibits a unique pseudogap phase below $T^* = 45$ K, recently probed with inelastic neutron scattering. This phase has been attributed to a possible preformation of Cooper pairs. We present detailed NMR results, including ^{75}As and ^{195}Pt spectra as well as T_1 measurements. These experiments reveal a drop of spin fluctuations just below T^* with a hysteresis in temperature, associated with the emergence of the pseudogap phase. Interestingly, no anomaly at T_c is found. At 3 K, a peak in the T_1 relaxation rate appears, until $1/T_1$ eventually vanishes at lower temperatures. This behavior is persistent in large magnetic fields up to 17 T. To interpret these results, scenarios including magnetic order below T^* are quite unprobable, since Korringa law is well complied at higher temperatures and no magnetic order is found in μSR. However, the origin of the unique behavior remains unclear for now.

TT 19.24 Mon 15:00 Poster D

Crystal growth of YFe_2Ge_2 and the dependence of its superconducting properties on sample preparation — •Jiasheng Chen[1], Konstantin Semeniuk[1], Zhuo Feng[2], Pascal Reiss[1], Philip Brown[1], Giulio Lampronti[3], and Malte Grosche[1] — [1]Cavendish Lab., Cambridge, UK — [2]London Centre of Nanotechnology, UCL, London, UK — [3]Dept. of Earth Sciences, Cambridge, UK

The d-electron system YFe_2Ge_2 exhibits an unusually high Sommerfeld ratio of specific heat capacity of C/T $\sim$ 100 mJ/(molK^2), signaling strong electronic correlations. Evidence of superconductivity has been reported in polycrystals and in flux-grown single crystals [1] with residual resistance ratios (RRR) of the order of 50, but these samples show no thermodynamic signatures of a bulk superconducting transition. We find that by combining (i) a prereaction of YFe_2, (ii) careful control of nominal composition, and (iii) subsequent annealing procedures, the polycrystalline YFe_2Ge_2 samples grown using a radio-frequency (RF) induction furnace can reach RRR values $\sim$ 200 with resistive superconducting transitions temperatures of around 1.85 K. This new generation of sample displays clear heat capacity anomalies as well as nearly 100% diamagnetic screening, confirming the bulk nature of its superconductivity.[2] We present details of the sample preparation and characterization and discuss the correlation between nominal composition and superconductivity.

[1] Y. Zou *et al.*, Physica Status Solidi (RRL) **8**, 928 (2014)
[2] J. Chen *et al.*, arXiv:1507.01436v2.

TT 19.25 Mon 15:00 Poster D

Superconductors in Non–Equilibrium: Higgs Oscillations and Induced Superconductivity — •Nikolaj Bittner[1], Holger Krull[1,2], Andreas Schnyder[1], Takami Tohyama[3], and Dirk Manske[1] — [1]Max–Planck–Institut für Festkörperforschung, D–70569 Stuttgart, Germany — [2]Lehrstuhl für Theoretische Physik, Technische Universität Dortmund, D–44221 Dortmund, Germany — [3]Department of Applied Physics, Tokyo University of Science, Tokyo 125–8585, Japan

Nonequilibrium pump–probe time–domain spectroscopy opens new perspectives in studying the dynamical properties of the strongly correlated electron systems. In particular, new effects, such as transient superconductivity [1] or Higgs oscillations of the superconducting condensate [2], can be obtained. Using various methods we present a theoretical study of the nonequilibrium dynamics in superconductors. Firstly, within the framework of the density matrix formalism we study Higgs oscillations in superconductors, which allow to detect the properties of the superconducting condensate as a function of time. For two–band superconductors the interplay between the phase (Leggett) and amplitude (Higgs) modes is analyzed in detail and new predictions are made. Secondly, employing the time–dependent Lanczos algorithm to the one–dimensional extended Hubbard model we observe appearance of a transient Meissner effect, which is a fingerprint of the induced superconductivity.

[1] S. Kaiser et al., PRB **89** , 184516 (2014)
[2] R. Matsunaga et al., PRL **111**, 057002 (2013)

TT 19.26 Mon 15:00 Poster D

Topological surface currents in chiral d-wave superconductors — •Wenbin Rui and Andreas P. Schnyder — Max-Planck-Institut für Festkörperforschung

Motivated by the locally non-centrosymmetric superconductor SrPtAs, the surface states of a multi-band chiral d-wave superconductor are investigated by using a tight-binding model which exhibits two point nodes. These gap closing points realize Weyl nodes that are protected by a nonzero Chern number. The nontrivial topology of this chiral d-wave superconductor manifests itself at the surface in terms of zero-energy arc states that connect the projected Weyl points in the surface Brillouin zone. By self-consistently solving Bogoliubov-de Gennes equations, we determine the spin and orbital character of the surface states. Moreover, we compute the spontaneous spin and charge currents at the surface of the superconductor, which arise due to the nontrivial topology and the strong spin-orbit interaction. We find that the currents are coupled to the chirality of the superconductor and show that they give rise to a small spin polarization at the surface, which could be measured by scanning SQUID microscopy.

TT 19.27 Mon 15:00 Poster D

Casimir forces between two impurities in a lattice — Dmitry Efremov[1], •Andrei Pavlov[1], and Jeroen van den Brink[1,2] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Dresden, Germany — [2]Department of Physics, Technical University Dresden, Dresden, Germany

We considered an interaction of impurities due to phonon exchange, leading to a long-range interaction, which behaves like Casimir forces. The contribution of virtual phonons is calculated by exact diagonalization of phonon operators on finite-sized lattices and by consideration of diagrams, describing exchange of phonons up to the second order of the perturbation theory, in an inverse space independently. The obtained results are consistent with good precision. The phonon interaction leads to attraction of impurities, but it is not strong enough for causing phase separation of the impurities inside a lattice both at zero and non-zero (but still small) temperatures.

TT 19.28 Mon 15:00 Poster D

Magneto-optical Kerr-effect at low temperatures: Investigation of superconductor/ferromagnet heterostructures — •Patrick Zahn[1,2], Claudia Stahl[1], Stephen Ruoss[1], Joachim Gräfe[1], Jonas Bayer[1,2], Gisela Schütz[1], and Joachim Albrecht[2] — [1]Max Planck Institute for Intelligent Systems, Heisenbergstraße 3, 70569 Stuttgart, Germany — [2]Institute for Innovative Surfaces FINO, Aalen University, Beethovenstraße 1, 73430 Aalen, Germany

With XMCD microscopy it is possible to visualize the critical current density of the superconductor YBCO with high spatial resolution [1,2]. Therefore, soft magnetic CoFeB is introduced as sensor layer. The magnetic stray fields of the supercurrents lead to a local reorientation of the magnetic moments in the ferromagnet, which are then imaged via X-ray microscopy. These experiments have to be carried out at the scanning x-ray microscope MAXYMUS at the synchrotron Bessy II in Berlin. For that purpose pre-characterization of the sensor is highly desirable: Magnetic interactions between the superconductor and the ferromagnetic sensor layer have been investigated at low temperatures using Kerr-effect measurements. Therefore hysteresis loops are obtained by a sophisticated magnet and field ramping setup within the NanoMOKE3 system [3]. The results are used to optimize the ferromagnetic sensor layer for XMCD microscopy of superconductors.

[1] C. Stahl et al., PRB **90**, 104515 (2014)
[2] S. Ruoß et al., APL **106**, 022601 (2015)
[3] J. Gräfe et al., Rev. Sci. Instrum. **85**, 023901 (2014)

TT 19.29 Mon 15:00 Poster D

Boosting the superconducting spin valve effect in a metallic superconductor/ferromagnet heterostructure — •Pavel Leksin[1,2], Andrey Kamashev[2], Joachim Schumann[1], Vladislav Kataev[1], Jürgen Thomas[1], Bernd Büchner[1,3], and Ilgiz Garifullin[2] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 Dresden, Germany — [2]Zavoisky Physical-Technical Institute, Russian Academy of Sciences, 420029 Kazan, Russia — [3]Technical University Dresden, D-01062 Dresden, Germany

We demonstrate a crucial role of the morphology of the superconducting layer for the operation of the multilayer S/F1/F2 spin valve. For that, we studied two types of superconducting spin valve heterostructures, with a rough and with a smooth superconducting layer, respectively, with transmission electron microscopy in combination with transport and magnetic characterization. We have found that the quality of the S/F interface is not critical for the S/F proximity effect as regards the suppression of the critical temperature of the S layer. However, it appears to be of a paramount importance for the performance of the S/F1/F2 spin valve. The magnitude of the conventional superconducting spin valve effect significantly increases, when the morphology of the S layer is changed from the type of overlapping islands to a smooth one. We attribute this drastic effect to a homogenization of the Green function of the superconducting condensate over the S/F interface in the S/F1/F2 valve with a smooth S layer surface.

TT 19.30 Mon 15:00 Poster D

Microwave spectroscopy and electronic transport properties of ferromagnetic Josephson junctions and superconducting spin-valves — Marcel Thalmann, Marcel Rudolf, and •Torsten Pietsch — Zukunftskolleg & Department of Physics, University of Konstanz, Universitätsstraße 10, 78464 Konstanz, Germany

Hybrid superconducting nanostructures recently attracted tremendous interest, due to their great potential in dissipation-less spin-electronics with unprecedented switching rates. The practical realisation of such devices, however, requires a complete understanding of the transfer and dynamics of spin- and charge currents between superconducting (S) and ferromagnetic (F) circuit elements, as well as the coupling between spin- and charge degrees of freedom in these systems. We investigate novel transport phenomena in superconductor-ferromagnet hybrid nanostructures under non-equilibrium conditions. Microwave spectroscopy is used to elucidate fundamental questions related to the complex interplay of competing order parameters and the question of relaxation mechanisms of non-equilibrium distributions with respect to spin, charge and energy. Recent experiments on two complimentary device structures are discussed: I) in diffusive S/F/S Josephson junctions with non-sinusoidal current-phase relationship and II) local and non-local transport measurements and microwave spectroscopy in F/S/F lateral spin-valves.

TT 19.31 Mon 15:00 Poster D

Superconducting Spin-Triplet-MRAM with Infinite Magnetoresistance Ratio — •Daniel Lenk[1], Roman Morari[1,2,3], Vladimir I. Zdravkov[1,2,4], 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[1,3], and Reinhard Tidecks[1] — [1]Institut für Physik, Universität Augsburg, D-86159 Augsburg, Germany — [2]D. Ghitsu Institute of Electronic Engineering and Nanotechnologies ASM, Academiei Str. 3/3, MD2028 Kishinev, Moldova — [3]Solid State Physics Department, Kazan Federal University, 420008 Kazan, Russia — [4]Present Address: Institute of Applied Physics and Interdisciplinary Nanoscience Center, Universität Hamburg, Jungiusstraße 9A, D-20355 Hamburg, Germany

We fabricated a nanolayered hybrid superconductor-ferromagnet spin-valve structure, i.e. the superconducting transition temperature of this structure depends on its magnetic history. The observed spin-valve effect is based on the generation of the long range odd in frequency triplet component, arising from a non-collinear relative orientation of the constituent ferromagnetic layers. We investigated the effect both as a function of the sweep amplitude of the magnetic field, determining the magnetic history, and the applied transport current. Moreover, we demonstrate the possibility of switching the system from the normal o

the superconducting state by applying field pulses, yielding an infinite magnetoresistance ratio.

TT 19.32 Mon 15:00 Poster D

Measurement of the Magnetic Penetration Depth in p-Doped Superconducting Diamond Films — •Lorenz Fuchs[1], Markus C.P. Brunner[1], Ina Schneider[1], Klaus Kronfeldner[1], Jessica Bousquet[2], Etienne Bustarret[2], and Christoph Strunk[2] — [1]University of Regensburg — [2]Institut Néel, Grenoble

Boron-doped diamond becomes superconducting once a critical doping concentration of $4.5 \times 10^{20} cm^{-3}$ is reached [1]. Mutual inductance measurements with a two-coil setup have been performed to determine the magnetic penetration depth $\lambda(T)$, which is a measure for the superfluid stiffnes $\theta \sim 1/\lambda^2(T)$. Two superconducting p-doped diamond films with thicknesses of 145nm and 345nm were investigated. At low temperatures these values agree reasonably with the values expected within BCS-theory using T_c, carrier density and mean free path determined from electric transport measurements. Magnetic penetration depths of $3.7\mu m$ for the thinner and $2.6\mu m$ for the thicker film have been found. λ decreases and accordingly θ increases with increasing film thickness. On the other hand, the superfluid stiffness drops by a factor of 2 or even more at $T_c/2$, i.e., much faster than expected from BCS-theory, but remains finite between $T_c/2 < T < T_c$. At present it is unclear, whether this behavior results from the proliferation of phase fluctuations already far below T_c or from a spatial inhomogeneity of the films.

TT 19.33 Mon 15:00 Poster D

Spin-dependent thermoelectric effects in superconductor-ferromagnet tunnel junctions — Stefan Kolenda[1], Christoph Sürgers[2], and •Detlef Beckmann[1] — [1]Institut für Nanotechnologie, Karlsruher Institut für Technologie — [2]Physikalisches Institut, Karlsruher Institut für Technologie

Recently, large thermoelectric effects were predicted to occur in superconductor-ferromagnet tunnel junctions with a spin-splitting of the density of states [1]. We have reported on the observation of these effects in samples where the spin splitting was induced by an applied magnetic field [2]. Here, we show results on samples where the spin splitting is enhanced by exchange coupling to the ferromagnetic insulator europium sulfide.

[1] Machon et al., PRL **110**, 047002 (2013);
Ozaeta et al., PRL **112**, 057001 (2014).
[2] Kolenda et al., arXiv:1509.05568.

TT 19.34 Mon 15:00 Poster D

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, Konstanz, Germany — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany

Experiments on superconductor-ferromagnet-systems have shown Cooper pairs tunneling through ferromagnetic layers, indicating Cooper pairs of equal spin, thus corresponding to a long-range triplet proximity effect [1]. Most experimental evidence for triplet superconductivity comes from observations of the thickness dependence of the Josephson current through a ferromagnetic barrier, but there is an increasing interest in obtaining direct spectroscopic evidence [2].

This project aims to analyze the DOS of thin films of the ferromagnetic insulator europium sulfide on superconducting aluminum or vice versa, using a scanning tunneling microscope in spectroscopy mode 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 and interpret our findings based on the diffusive theory [3,4]

[1] F. S. Bergeret, PRL **86**, 4096 (2001)
[2] F. Hübler, PRL **109**, 87004 (2012)
[3] P. Machon, PRL **110**, 047002 (2013)
[4] J. Linder, PRB **81**, 214504 (2010)

TT 19.35 Mon 15:00 Poster D

Superconducting Atom Chips — Christoph Hufnagel[2], Deshui Yu[2], Chin Chean Lim[2], Alessandro Landra[2], Chee Howe Ew[2], and •Rainer Dumke[1,2] — [1]Division of Physics & Applied Physics, School of Physical & Mathematical Sciences, Nanyang Technological University, Singapore — [2]Centre for Quantum Technologies, National University of Singapore, Singapore

Recently superconducting atom chips have generated a lot of interest due to their attractive properties, such as the Meissner effect for type-I superconductors and vortices for type-II superconductors. Thermaland technical noise in proximity to superconducting surfaces have been shown both theoretically and experimentally to be significantly reduced compared to conventional atom chips. Superconducting atom chips have the potential to coherently interface atomic and molecular quantum systems with quantum solid state devices. I will present recent developments in our superconducting atom chip experiment.

TT 19.36 Mon 15:00 Poster D

Interplay between Superconductivity and Coulomb Blockade — •Thomas Lorenz, Susanne Sprenger, and Elke Scheer — Universität Konstanz, Germany

Studying the interplay between superconductivity and Coulomb blockade (CB) can be achieved by investigating an all superconducting single electron transistor (SSET) consisting of an island coupled to the leads by two tunneling contacts. The majority of experiments performed so far were using superconducting tunnel contacts made from oxide layers, in which multiple Andreev reflections (MAR) can be excluded.

Using a mechanically controlled break junction (MCBJ) made of aluminum enables tuning the contributions of MAR in one junction continuously and thereby addressing different transport regimes within the same sample. Our results offer the possibility to attribute particular features in the transport characteristics to the transmission probabilities of individual modes in the MCBJ contact. We discuss our findings in terms of dynamical CB, SSET behaviour and MAR when continuously opening the MCBJ from the fully closed state to a tunneling contact.

TT 19.37 Mon 15:00 Poster D

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

Single C_{60} molecules deposited on an ultrathin oxide film on Nb(110) were investigated using a low-temperature scanning tunnelling microscope. Spectroscopy of the differential conductance (dI/dV) in the tunnelling range indicates proximity-induced superconductivity in junctions comprising the oxide layer as well as single C_{60} molecules. Andreev reflection is enhanced upon controlled fabrication of tip-surface contacts. With decreasing electrode separation the Bardeen-Cooper-Schrieffer energy gap gradually evolves into a zero-bias peak in dI/dV spectra reflecting the spectroscopic signature of Andreev reflection. The current-voltage characteristics of the tunnelling and contact junctions are well described by the Blonder-Tinkham-Klapwijk theory. Our spectroscopic data evidence the influence of the electrodes' atomic-scale structure on electron transport across normal metal-superconductor interfaces.

Funding by the Deutsche Forschungsgemeinschaft through KR 2912/10-1 is acknowledged.

TT 19.38 Mon 15:00 Poster D

Perturbation theory for a single-level quantum dot connected to superconducting leads — •Vladislav Pokorný[1], Martin Žonda[2], Václav Janiš[1], and Tomáš Novotný[2] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 18221 Praha, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University in Prague, Ke Karlovu 5, 12116 Praha, Czech Republic

The zero-pi quantum phase transition in a single-level quantum dot attached to two superconducting leads is studied via the perturbation expansion in the interaction strength. We use the Nambu formalism and the standard many-body diagrammatic representation of the impurity Green functions to formulate the self-consistent perturbation expansion. We show that at zero temperature second order of the expansion in its spin-symmetric version yields a good agreement with the numerical renormalization group calculations for the position of the phase boundary as well as for the parameters in the zero phase. We present results for phase diagrams, level occupation, induced local superconducting gap, Josephson current and energy of the Andreev bound states. We also show the agreement of the second order perturbation method with the existing experimental data.

TT 19.39 Mon 15:00 Poster D

Towards quantum signatures in a swept-bias Josephson junction — •Harald Losert, Karl Vogel, and Wolfgang P. Schle-

ich — Institut für Quantenphysik and Center for Integrated Quantum Science and Technology (IQ^{ST}), Universität Ulm, D-89069 Ulm, Germany

Josephson junctions are one of the best examples for the observation of macroscopic quantum tunneling. The phase difference in a current-biased Josephson 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.
Quantum mechanically, the escape from the washboard potential can be explained as tunneling from the ground state, or an excited state. However, it has been shown [1][2], that in the case of periodic driving the experimental data for quantum mechanical key features, e.g. Rabi oscillations or energy level quantization, can be reproduced by a completely classical description.
Motivated by this discussion, we investigate a swept-bias Josephson junction in the case of a large critical current. In particular, we contrast the switching current distributions resulting from a quantum mechanical and classical description of the time evolution.
[1] M. Marchese *et al.*, Eur. Phys. J. Special Topics **147**, 333 (2007)
[2] J. A. Blackburn *et al.*, PRB **85**, 104501 (2012)

TT 19.40 Mon 15:00 Poster D

Low frequency dielectric properties of amorphous AlO_x — •Arnold Seiler, Saskia Meissner, Hannes Rotzinger, and Georg Weiss — Physikalisches Institut, Karlsruher Institut für Technologie

Tunneling systems (TS) are well known to dominate the low temperature properties of amorphous and disordered solids. In superconducting circuits they interact with resonators and qubits and limit their quality factors and coherence times.

We go further and want to know, whether the TS in the dielectric material used in these circuits were distributed according to the standard tunneling model. Therefore we investigate different plate capacitor geometries containing the same dielectric AlO_x as used in qubits. With resonators and large capacitors we cover a broad frequency range to probe the dielectric response of the TS.

Here we present the low frequency measurements on capacitors of 0.25 mm^2 and 1 mm^2 down to 15 mK. Surprisingly the application of a magnetic field leads to a dramatic change of the dielectric response. In respect to glasses a similar effect is known the elastic response of from superconducting metallic glasses but was not expected in the dielectric behavior of an insulating material.

TT 19.41 Mon 15:00 Poster D

Dielectric susceptibility measurements of amorphous AlO_x using superconducting resonators — •Saskia Meissner, Arnold Seiler, Hannes Rotzinger, and Georg Weiss — Physikalisches Institut, KIT Karlsruhe

The performance of superconducting circuits like Quantum Bits, SQUIDs and resonators is well known to be limited due to dielectric loss caused by tunneling systems (TS). They are a source of noise, energy loss and decoherence due to their coupling to electric fields.

Measurements of individual TS coherently coupled to a Josephson Junction (JJ) already indicate their broad energy distribution in the range of qubit frequencies.

Here we present measurements of the low temperature dielectric response of thin film AlO_x in a wide frequency range in order to extract the spectral distribution of TS for a comparison with the standard tunneling model. AlO_x films are fabricated in the same way as those of JJ implemented as plate capacitors. Direct capacitance measurements and selected resonances of lumped element superconducting resonators offer excitation frequencies from the kHz range up to the GHz range where superconducting quantum circuits are commonly operated.

TT 19.42 Mon 15:00 Poster D

NbN-AlN-NbN Josephson junctions on different substrates — •Michael Merker, Christian Bohn, Marvin Völlinger, Konstantin Ilin, and Michael Siegel — KIT, Karlsruhe, Deutschland

Josephson junction technology is important for the realization of high quality cryogenic devices such as SQUIDs, RSFQ or SIS-mixers. The material system based on NbN/AlN/NbN tri-layer has gained a lot of interest, because it offers higher gap voltages and critical current densities compared to the well-established Nb/Al-AlOx/Nb technology. However, the realization of high quality Josephson junctions is more challenging. We developed a technology of Josephson junctions on a variety of substrates such as Silicon, Sapphire and Magnesium oxide and compared the quality parameters of these junctions at 4.2 K.The gap voltages achieved a range from 4 mV (for the junctions on Si) to 5.8 mV (in case of MgO substrates) which is considerably higher than those obtained from Nb based Josephson junctions. Another key parameter is the ratio of the subgap resistance to the normal state resistance. This so-called subgap ratio corresponds to the losses in a Josephson junction which have to be minimized. So far, subgap ratios of 26 have been achieved. Further careful optimization of the deposition conditions is required to maximize this ratio, The details of the optimization of technology and of characterization of NbN/AlN/NbN junctions will be presented and discussed.

TT 19.43 Mon 15:00 Poster D

Investigation of a Josephson junction based parametric amplifier — •Patrick Winkel[1], Martin Weides[1,2], and Alexey V. Ustinov[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe — [2]Materials Science in Mainz, Johannes Gutenberg-Universität Mainz, 55128 Mainz

We design, fabricate and experimentally investigate a parametric amplifier based on the nonlinear inductance of Josephson junctions. Our design is rather conventional and based on a strongly coupled coplanar waveguide quarter-wave resonator terminated by a SQUID. The SQUID inductance depends periodically on the enclosed magnetic flux inside the loop. This tunable nonlinear inductance is used to adjust the resonance frequency of the whole device. We replace the single SQUID with a series array of SQUIDs to decrease the effective nonlinearity and to increase the dynamic range without affecting the bandwidth. The required pump tone is introduced through a separate flux line by applying an rf-drive. For a critical pump power and detuning between pump and resonance frequency, the system reaches a bifurcation regime. Close to this critical point, the response of the system is highly sensitive to small perturbations, which are intentionally introduced by the signal fed into the amplifier.

TT 19.44 Mon 15:00 Poster D

Dual-circuit Hamiltonian construction for superconducting elements in high-impedance environments — •Jascha Ulrich and Fabian Hassler — JARA-Institute for Quantum Information, RWTH Aachen University

Devoret has popularized a simple and easy-to-use recipe for the Hamiltonian description of arbitrary superconducting circuits involving nonlinear Josephson inductances in terms of node fluxes. In the last years, phase slip elements, nonlinear capacitors electromagnetically dual to the Josephson inductances, have attracted a lot of interest. Unfortunately, Devoret's construction cannot be applied directly to circuits involving nonlinear capacitors. Here, we give a simple dual formulation of Devoret's recipe in terms of loop charges which is well suited for the description of phase slip elements and is particularly timely in view of recent experimental advances in their realization using superconducting nanowire. However, we argue that our construction is not restricted to phase slip elements, but more generally useful for the effective description of Josephson junctions embedded in high-impedance environments. As an example, we illustrate how our formalism can give new physical insights and facilitate the phenomenological modeling of the fluxonium qubit and the 0-π qubit.

TT 19.45 Mon 15:00 Poster D

Josephson junctions array resonators — •Oscar Gargiulo, Phani Muppalla, Iman Mirzaei, and Gerhard Kirchmair — Institute for Quantum Optics and Quantum Information, Innsbruck, Austria

We present an experimental analysis of the self- and cross-Kerr effect of extended plasma resonances in Josephson junction chains. The chain consists of 1600 individual junctions and we can measure quality factors in excess of 10000. The Kerr effect manifests itself as a frequency shift that depends linearly on the number of photons in a resonant mode. By changing the input power we are able to measure this frequency shift on a single mode (self-kerr). By changing the input power on another mode while measuring the same one, we are able to evaluate the cross-kerr effect. We can measure the cross-Kerr effect by probing the resonance frequency of one mode while exciting another mode of the array with a microwave drive.

TT 19.46 Mon 15:00 Poster D

Single crystal $Bi_2Sr_2CaCu_2O_8$ structures as THz-emitters — •Raphael Wieland[1], Fabian Rudau[1], Julian Langer[1], Nickolay Kinev[2], Jie Yuan[3], Ya Huang[3,4], Min Ji[3,4], Xianjing Zhou[3,4],

Akira Ishii[3], Peiheng Wu[4], Takeshi Hatano[3], Huabing Wang[3,4], Valery Koshelets[2], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Physikalisches Institut and Center for Collective Quantum Phenomena in LISA$^+$, Universität Tübingen, Tübingen, Germany — [2]Kotel'nikov Institute of Radio Engineering and Electronics, Moscow, Russia — [3]National Institute for Materials Science, Tsukuba, Japan — [4]Research Institute of Superconductor Electronics, Nanjing University, Nanjing, China

By means of Josephson Junctions (JJs) one can easily convert a dc voltage into high-frequency electromagnetic radiation. The high-Tc superconductor $Bi_2Sr_2CaCu_2O_8$ (BSCCO) has a layered crystal structure in such a way that JJs form intrinsically. This allows to fabricate hundreds of stacked junctions with reasonable effort. Terahertz emission can be observed at relatively low bias currents but also at higher input power. Emission frequencies from 0.4 to 2.4 THz have been measured. A hot spot forms at high bias currents with effect on both intensity and linewidth of the THz emission.BSCCO mesas probably act as a cavity for electromagnetic standing waves that synchronize all junctions in the stack. We investigated hotspot formation and THz emission using a combination of transport measurements, low temperature scanning laser microscopy and electromagnetic wave detection via a superconducting receiver.

TT 19.47 Mon 15:00 Poster D

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

Semiconductor single electron pumps allow the controlled transport of electrons with a frequency f (about 1 GHz) which results in a current ($I = e \times f$) in the range of about 0.1 nA. However, since the pumping mechanism is prone to errors due to the stochastic nature of the transport mechanism, the accuracy of these devices is limited (0.2 ppm at the moment). We developed a method to detect and account the errors of these pumps. To realize this error detection we integrate several electron pumps in a serial circuit with intermediate charge nodes between them, so the pumping errors can be detected by monitoring the charge of the nodes. As ultra-sensitive charge detectors we used superconducting Al single electron transistors (SETs) capacitively coupled to the intermediate nodes. To increase the readout bandwidth of the SET and, therefore detect errors at relatively high rate, we put the SETs in resonant tank circuits and measured the reflectance from these resonators. With such an integrated device we can achieve a significant improvement in accuracy. The measurement setup and the progress of counting measurements with such a RF-SET will be reported.

TT 19.48 Mon 15:00 Poster D

Microfabricated Thick Proximity Bi-layers as Sensors for Magnetic Penetration Thermometers (MPTs) — •Jeschua Geist, Daniel Hengstler, Andreas Fleischmann, Loredana Gastaldo, Sebastian Kempf, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg University, Germany

Microcalorimeters with inductively coupled temperature sensors like metallic magnetic calorimeters (MMC) are widely used for many applications.Whereas MMCs use dilute paramagnetic alloys as temperature sensors operated at temperatures below 30 mK, magnetic penetration depth thermometers (MPT) make use of the steep temperature dependence of the magnetic penetration depth of a superconducting sensor, potentially offering improved temperature sensitivity at higher and hence easier accessible temperature. Operated below T_c of the sensor material, the temperature change upon the absorption of an X-ray in the detector leads to a change of the magnetic flux density $B(\mathbf{r})$ inside the superconducting sensor and in its vicinity which is detected using a SQUID and serves as a measure of the absorbed energy.

So far we studied the elemental superconductors, Hf, Ir, Ti, Al, Nb, and recently thick proximity bilayers of Al and Au, promising a large range of operational temperatures. We also demonstrated that the penetration of flux lines and the hysteresis of the magnetisation can be engineered by patterning the superconducting sensor layer in form of discs or stripes. We present data on thick bilayers, allowing to tune not only T_c, but also the transition width and therefore the dynamic range, with various geometries and corresponding numerical simulations.

TT 19.49 Mon 15:00 Poster D

Fabrication of the 4k-Pixel Molecule Camera MOCCA and its Integration into the Cryogenic Storage Ring CSR — •L. Gamer[1], C. Enss[1], A. Fleischmann[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 at the Max Planck Institute for Nuclear Physics in Heidelberg is able to store heavy molecular ions in their rotational and vibrational ground states. In a near future electron-ion-interactions, such as the dissociative recombination, will be investigated in laboratory environment at conditions that are close to those in cold interstellar plasmas. To reconstruct the full kinematics of these processes, a position and energy sensitive coincident detection of multiple reaction products is necessary. We recently designed and fabricated MOCCA, a 4k-pixel molecule camera based on magnetic calorimeters with a detection area of 45 mm × 45 mm segmented into 64×64 absorbers. We present the detector design and microfabrication as well as the plans for integrating MOCCA and its ^{3}He/^{4}He dilution refrigerator into CSR.

TT 19.50 Mon 15:00 Poster D

Microwave SQUID multiplexing of large MMC detector arrays — •M. Keller, M. Wegner, S. Kempf, L. Gastaldo, A. Fleischmann, and C. Enss — Kirchhoff-Institute for Physics, Heidelberg University

Metallic magnetic calorimeters (MMCs) are the devices of choice for many spectroscopic applications since they provide a very good energy resolution, a very fast intrinsic signal rise time as well as an excellent linearity. While single MMCs or small detector arrays are typically read out by dc-SQUIDs, the readout of very large arrays requires a cryogenic multiplexing technique to limit the parasitic heat load to the cold stage of the cryostat, the system complexity as well as cost.

A very promising approach for the readout of very large MMC arrays is microwave SQUID multiplexing. Here, the initial detector signal is transduced into a resonance frequency shift of a related superconducting $\lambda/4$ microwave resonator by means of a non-hysteretic, unshunted rf-SQUID. By coupling many resonators - each with unique resonance frequency - to a common transmission line, this frequency domain multiplexing technique allows for the readout of hundreds or thousand pixels with only one HEMT amplifier and two coaxial cables.

In this contribution we discuss the performance of a recently developed 64 pixel MMC detector array that is read out by means of an on-chip multiplexer. For the very first time we demonstrate the simultaneous readout of two MMCs by means of a microwave SQUID multiplexer.

TT 19.51 Mon 15:00 Poster D

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

Two-stage current-sensing dc-SQUIDs are presently the devices of choice to read out single-channel magnetic microcalorimeters (MMCs) since they provide quantum-limited noise performance, large system bandwidth and are compatible with operation temperatures well below 100 mK. However, it is very well known that parasitic inductances in the SQUID input circuitry lead to a reduction of the signal size of the detector and that SQUID noise often sets a limit to the energy resolution. In order to minimize these effects, we develop two-stage current-sensing dc-SQUIDs optimized for MMC readout as well as dc-SQUIDs suited for direct temperature sensor readout.

In this contribution we discuss our SQUID designs including single second-order gradiometric SQUIDs, N-SQUID series arrays as well as SQUIDs with meander-shaped SQUID inductance that are eligible for direct temperature sensor readout. We show that our SQUIDs exhibit exceptional small low-frequency excess flux noise and are hence very well suited for MMC readout. We further present an integrated setup in which detector and SQUID are located on the same chip to maximize the coupling efficiency of the superconducting flux transformer. Finally, we discuss experimental data of a detector setup with direct temperature sensor readout and prove that this strategy should allow for reaching a sub-eV energy resolution.

TT 19.52 Mon 15:00 Poster D

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

We develop microfabricated, energy dispersive particle detector arrays based on metallic magnetic calorimeters (MMCs) for high resolution x-ray spectroscopy to challenge bound-state QED predictions. Our MMCs are usually operated below 30 mK and use a paramagnetic temperature sensor placed in a weak magnetic field, read-out by a SQUID, to measure the energy deposited by single x-ray photons. We discuss the physics of MMCs, their microfabrication and the detector performances of three detector arrays together with the cryogenic setups used for their operation. Two of these arrays, maXs-20 and maXs-200, are linear 1x8 arrays optimized for x-rays with energies up to 20 and 200 keV respectively. maXs-20 achieved an energy resolution of 1.6 eV for 6 keV x-rays and maXs-200 achieved an energy resolution of 45 eV for 60 keV x-rays. Both detectors already allowed to investigate excellent physics in several labs around the world. The third detector, the maXs-30, is our first 2d 8x8 pixel array prototype with an active detection area of 16 mm^2 and is optimized for x-rays up to 30 keV with an expected energy resolution below 6 eV when operated at 10 mK in a cryogen free $^3He/^4He$-dilution refrigerator at the tip of a 40 cm long cold finger.

TT 19.53 Mon 15:00 Poster D

Optimization of metallic magnetic calorimeters with embedded ^{163}Ho — •Ch. Fischer[1], H. Dorrer[2], Ch. E. Düllmann[2], K. Eberhardt[2], Ch. Enss[1], A. Fleischmann[1], L. Gastaldo[1], C. Hassel[1], D. Hengstler[1], S. Hähnle[1], K. Johnston[3], S. Kempf[1], T. Kieck[2], M. Krantz[1], U. Köster[4], F. Schneider[2], A. Türler[5], M. Wegner[1], and K. Wendt[2] — [1]Kirchhoff-Institut für Physik, Heidelberg — [2]Johannes Gutenberg-Universität, Mainz — [3]Physics Department CERN, Geneva — [4]Institut Laue-Langevin, Grenoble — [5]Laboratory of Radiochemistry and Environmental Chemistry, Paul Scherrer Institut, Villigen

The Electron Capture in ^{163}Ho (ECHo) collaboration plans to reach sub-eV sensitivity on the electron neutrino mass by the analysis of high statistics of ^{163}Ho electron capture spectra. Large arrays of metallic magnetic calorimeters (MMCs) with enclosed ^{163}Ho read out using microwave SQUID multiplexing will be used for the measurement of the spectrum. With first prototypes of MMCs having the ^{163}Ho source ion-implanted in the absorbers, operated at 25 mK, an energy resolution ΔE_{FWHM} = 7.6 eV and a signal rise time τ = 130 ns have been achieved, paving the way to the first stage of the experiment (ECHo 1k). We present the optimization of MMCs and of the methods to embed the high purity ^{163}Ho source in detector absorbers. In particular we discuss how to define the optimal activity per pixel considering the limits coming from the allowed unresolved pileup fraction and from the additional contribution of detector heat capacity related to the magnetic moments of ^{163}Ho.

TT 19.54 Mon 15:00 Poster D

Development of phonon and photon detectors for rare events searches using scintillating crystals — •Felix Ahrens[1], Christian Enss[1], Andreas Fleischmann[1], Loredana Gastaldo[1], Clemens Hassel[1], Sebastian Hendricks[1], Sebastian Kempf[1], Yong-Hamb Kim[2], Martin Loidl[3], Xavier-François Navick[3], and Matias Rodrigues[3] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Deutschland — [2]Korea Research Institute of Standards and Science, Daejeon, Rep. of Korea — [3]Commissariat à l'énergie atomique, Saclay, France

The use of scintillating crystals in cryogenic experiments searching for neutrinoless double beta decay and for direct interaction of dark matter particles allows for an efficient background reduction due to particle discrimination. We develop phonon and photon detectors based on metallic magnetic calorimeters (MMCs) to perform simultaneous measurements of heat and light generated by the interaction of a particle in a scintillating crystal. As designed we expect for the phonon sensor an energy resolution of $\Delta E_{FWHM} < 100$ eV and a signal rise time $\tau < 200\,\mu$s whereas for the photon detector we expect $\Delta E_{FWHM} < 5$ eV and $\tau < 50\,\mu$s. We discuss the design and the fabrication of these detectors and present recent results.

TT 19.55 Mon 15:00 Poster D

Study of single-spiral superconducting nanowire single-photon detectors in magnetic fields — •Ilya Charaev[1], Robert Lusche[2], Alexei Semenov[2], Konstantin Ilin[1], and Michael Siegel[1] — [1]Institut für Mikro- und Nanoelektronische Systeme, KIT, Hertzstraße 16, 76187 Karlsruhe — [2]Institut für Optische Sensorsysteme, DLR, Rutherfordstraße 2, 12489 Berlin

We present single-spiral superconducting nanowire single-photon detectors (SNSPD) with critical currents I_c and detection efficiencies which were improved by applying a magnetic field B. The structures were made from 100 nm wide and 5 nm thick superconducting NbN nanowires. We investigated circular spirals and rectangular spirals, both with a pitch of 150 nm and superconducting transition temperature about 12 K. We achieved a more than 10 percent increase of the critical current in magnetic fields for rectangular spirals. Contrary, circular spirals showed fully symmetrical I_c(B) dependencies, with the maximum of I_c at zero field.

The detection efficiency of spirals has been studied in a wide spectral range and in magnetic fields up to 500 mT. In circular spirals, the rates of light and dark counts were symmetric in magnetic fields at all achievable experimental conditions. In rectangular spirals, photon count rates were asymmetric with the minima at opposite direction of the field than the maximum of I_c. Dark count rates in these structures also demonstrated asymmetric behavior with respect to the magnetic field for the whole range of applied bias currents.

TT 19.56 Mon 15:00 Poster D

Influence of back reflections on the detection efficiency of superconducting nanowire single-photon detectors on GaAs — •Ekkehart Schmidt[1], Mario Schwartz[2], Thomas Herzog[2], Konstantin Ilin[1], Michael Jetter[2], Peter Michler[2], and Michael Siegel[1] — [1]Institut für Mikro- und Nanoelektronische Systeme (IMS), Karlsruher Institut für Technologie, Hertzstrasse 16, 76187 Karlsruhe, Germany — [2]Institut für Halbleiteroptik und funktionelle Grenzflächen (IHFG), Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

In an on chip quantum photonic device, which consists of quantum dots, a waveguide based logic and a SNSPD, the quantum dots are conveniently excited by a laser beam. Backside reflection of these excitation photons can lead to their detection by the SNSPD and therefore to malfunction of the whole photonic circuit. We studied the effect of back reflections at the substrate/sample-holder interface on the detection properties of NbN SNSPDs on a GaAs substrate with a 12 nm AlN buffer layer. The SNSPDs have a width of 120 nm, a thickness of 6 nm, a critical temperature of 9.9 K and a critical current density of 2.8 MA/cm^2 at 4.2K. Two identical SNSPDs were fabricated from the same NbN film at a distance of 50 μm from each other. One of these SNSPDs was covered with a bi-layer of 20 nm thick AlN and 110 nm thick Al to prevent top illumination, making it only sensitive to backscattered photons. Results of the study of the influence of backscattered photons on the optical response of the SNSPDs and possibilities to avoid them will be discussed in detail.

TT 20: Cryotechnique & Measuring Devices: Poster Session

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

TT 20.1 Mon 15:00 Poster D

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

Among the family of regenerative cryocoolers, Pulse Tube Coolers (PTCs) distinguish themselves from Gifford-McMahon- or Stirling coolers by the absence of cold moving parts inside the cold head. This features a long live operation with low vibration of the PTC and less maintenance compared to conventional cryocoolers - making them attractive for low noise applications. Since their invention, 4 K PTCs [1] have become an excellent alternative for "dry" cooling of cryogenic experiments without liquid helium ("wet") even below 4 K. Besides their advantages, PTCs - like all other regenerative cryocoolers - suffer from two intrinsic effects due to the periodic compression and expanding

cycles in the cold head: a periodic elastic deformation ("breathing") of the thin walled pulse- and regenerator-tubes, which leads to residual vibrations and a periodic variation in temperature. Here we present unique applications of double-staged 4 K PTC based cryostats. By adapting the cooling power to the requirement of the experiment, the intrinsic effects of the PTC are minimized. Further decoupling and damping of the mechanical and thermal variations provide an excellent environment even for cooling of sensitive devices.
[1] G. Thummes, C. Wang, C. Heiden, Cryogenics **38**, 337 (1998)

TT 20.2 Mon 15:00 Poster D

Low-Noise Pulse Tube Cryocooler near 5 K: development of a system for operation of optical detectors — •Matthias Vorholzer[1,2], Bernd Schmidt[1,2], Jens Falter[1], Marc Dietrich[1,2], André Schirmeisen[1,2], and Günter Thummes[1,2] — [1]TransMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany — [2]Institute of Applied Physics, Justus-Liebig-University, Giessen, Germany

Pulse tube cryocoolers (PTC) are, beside Gifford-McMahon and Stirling-cryocoolers, an option for "dry" cooling down to liquid helium temperatures. A unique feature of the PTC, the absence of a moving displacer in the cold head, reduces the required maintenance compared to other cryocoolers and allows a setup with low mechanical vibrations. While plenty of development aims towards high cooling powers, for many applications cooling powers below 100 mW near 4-5 K are already sufficient for operation.

In the framework of the BMBF joint project "SUSY" (SUperconducting optical sensors based on a compact cryogen-free SYstem platform) we are developing a low-noise 2-stage 5 K PTC for cooling of transition edge bolometers and single-photon detectors with an input power of 1 kW or less. Reducing the vibrations is critical for those sensors and can mainly be achieved by reducing the pressure oscillation and downsizing the cold head. With only 1 kW input power and a considerable reduction in size the oscillatory displacement of the cold head is significantly lowered compared to typical PTC.

Work supported by the German BMBF under grant no. 13N13444

TT 20.3 Mon 15:00 Poster D

Current Sensing Noise Thermometer with Cross Correlated Readout for Milli-Kelvin Temperatures — •Felix Mücke, Andreas Reifenberger, Marius Hempel, 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. We present the thermometer design and discuss the results of experimental tests, where we compared 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 expectations from the thermal model of the thermometer, which suggests that self heating should be marginal even at temperatures well below 1 mK.

TT 20.4 Mon 15:00 Poster D

Experimental aspects of the specific heat of superconductors derived from topological insulators — •Lionel Andersen, Oliver Breunig, Thomas Lorenz, and Yoichi Ando — II. Physikalisches Institut - Universität zu Köln, Germany

The expectation for topological superconductors to have an unconventional pairing symmetry makes them promising hosts for Majorana fermions. Recently the topological insulators Bi_2Se_3 (BS) and $(PbSe)_5(Bi_2Se_3)_6$ (PSBS) were reported to become superconducting when intercalating them with copper [1, 2]. Literature data of specific heat on both, Cu_xBS and Cu_xPSBS, indicate an unusual temperature dependence not described by standard BCS theory [2, 3]. This makes them promising candidates of topological superconductors but in order to clarify these issues it is necessary to perform c_p measurements below 250 mK using a $^3He/^4He$ dilution cryostat. Because c_p of superconductors becomes very small far below T_c the addendum contribution of the setup has to be minimized. This demand together with other complications e.g. nuclear Schottky contributions to c_p, leads to a drastic increase of the experimental effort. In this contribution experimental aspects of c_p measurements with respect to the topological superconductor materials will be discussed in detail.
[1] Y. S. Hor et al., PRL **104** 057001 (2010)
[2] Y. Ando et al., PRB **90** 220504 (2014)
[3] Y. Ando et al., PRL **106** 127004 (2011)

TT 20.5 Mon 15:00 Poster D

Low temperature measurements of thermal conductivity and thermal diffusivity of thin metal films using the 3ω method — •Sofia Blanter[1], Sasmita Srichandan[1], Denis Kochan[2], and Christoph Strunk[1] — [1]Institut für experimentelle und angewandte Physik, Universität Regensburg, Universitätstr. 31, 93053 Regensburg — [2]Universität Regensburg, Institut I - Theoretische Physik, Universitätsstraße 31, 93053 Regensburg

We present measurements of thermal conductivity and thermal diffusivity for thin suspended membranes. The measurements are performed on 500 nm thick SiN membranes using the 3ω method [1]. We pass an AC current at a frequency ω through a metal transducer on top of the membrane. This applied current generates an oscillating heat flux through the membrane. This will create a modulation on top of the measured voltage through the transducer, at a frequency of 3ω.

By depositing thin metal films on the backside of the membranes, we are able to obtain thermal properties for thin metal films once the plain membrane is characterized. We derive a model from the two-dimensional heat diffusion equation, which allows us to extract both the thermal conductivity and thermal diffusivity of the sample.
[1] D. Cahill and R. Pohl, PRB **35**, 4067 (1987).

TT 20.6 Mon 15:00 Poster D

Design of a vector magnetometer for three dimensional magnetization measurements — •Markus Kleinhans, Marco Halder, Christopher Duvinage, and Christian Pfleiderer — Physik-Department, Technische Universitaet Muenchen, 85748 Garching, Germany

In magnetically ordered systems, the fundamental order parameter is the magnetization which is, in general, a three dimensional pseudovector. However, conventional magnetometers record the projection of the moment along the applied magnetic field hence missing key information of systems with complex magnetic anisotropies. We report the design of a bespoke set of pickup coils for a vibrating sample magnetometer that allow simultaneous measurements of all three components of the magnetization for temperatures down to 3 K and in magnetic fields up to 9 T. We demonstrate the potential of this technique in a study of selected anisotropic ferromagnets, namely Co, $Nd_2Fe_{14}B$, and $SmCo_5$.

TT 21: Frontiers of Electronic Structure Theory: Focus on Topology and Transport (Joint session of DS, HL, MA, MM, O and TT organized by MM)

Time: Monday 15:45–17:45 Location: H51

TT 21.1 Mon 15:45 H51

Mechanism of Li intercalation/deintercalation into/from the surface of $LiCoO_2$ — •Ashkan Moradabadi and Payam Kaghazchi — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

$LiCoO_2$ is the most commonly used cathode material in Li-ion bat-

teries. In this work, we have investigated atomic and electronic structures, magnetic properties, formation energies, and energy barriers for the diffusion of Li in single vacancies, divacancies, and missing rows in bulk and surface of $LiCoO_2$. Our GGA-PBE results indicate that there is almost no energy barrier for the Li-ion deintercalation from the surface layer. Energy barrier for the Li-ion intercalation is also very small. However, we find that Li hopping in PBE+U is accompanied by electron hopping between nearby transition metal ions. Therefore a PBE+U barrier, which is for both Li hopping and charge hopping, is higher than the corresponding PBE barrier [1]. This study has implications in understanding the role of the surface in the rate capability of nanostructured $LiCoO_2$ cathodes of Li-ion batteries.

[1] Ashkan Moradabadi and Payam Kaghazchi, Mechanism of Li intercalation/deintercalation into/from the surface of $LiCoO_2$, Phys. Chem. Chem. Phys., 2015, 17, 22917-22922.

TT 21.2 Mon 16:00 H51

Potential-dependent mechanism of Li diffusion in Li_2S — •Ashkan Moradabadi[1,2] and Payam Kaghazchi[1] — [1]Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — [2]Institut für Materialwissenschaft, Fachgebiet Materialmodellierung, Technische Universitat Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt, Germany

Li-S batteries are promising candidates for large-scale applications such as electrical vehicles. However, the measured discharge capacity is often less than the theoretical one [1,2]. This is mainly due to the slow diffusion of Li through Li_2S shells formed on S_8 cores, which leads to an incomplete conversion of S_8 cores to Li_2S (the final product of lithiation of S_8). In the present work, using density functional calculation, we have investigated mechanism of Li diffusion in Li_2S. At low cell voltages (< 0.93 V), Li diffusion occurs via an exchange mechanism with a high energy barrier of 0.45 eV. However at higher cell voltages, Li diffusion takes place via a vacancy mechanism with a lower energy barrier of 0.27 eV. Our findings can explain the capacity fading in Li-S batteries at high operation rates.

[1] Liang, X.; Hart, C.; Pang, Q.; Garsuch, A.; Weiss, T.; Nazar, L. F.; A highly efficient polysulfide mediator for lithium-sulfur batteries. Nature Communications, 2015, 6, 5682.

[2] Wang, L.; Wang, Y.; Xia, Y.; A high performance lithium-ion sulfur battery based on a Li_2S cathode using a dual-phase electrolyte. Energy Environ. Sci. 2015, 8, 1551.

TT 21.3 Mon 16:15 H51

Extremely high magnetoresistance in topological insulator candidate LaBi — •Nitesh Kumar, Chandra Shekhar, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

Lanthanum monopnictides (LaX, X=N, P, As, Sb, Bi) have recently been predicted to be topological insulators, except LaN which is a topological semimetal. Inspired from this report we have studied the transport properties of LaBi. It has a simple rock salt-type structure with alternate La and Bi atoms arranged in all three directions. Temperature variation of resistivity at different magnetic fields follows Kohler's rule. Resistivity follows almost a parabolic relation with magnetic field without saturation, exhibiting a huge magnetoresistance (1.5 x10^5% at 2 K and 9 T). By employing two band model we calculate carrier density and mobility of electrons and holes which suggests that LaBi is a compensated system. We believe this to be responsible for high unsaturated MR in LaBi. We observe excellent Shubnikov-de Haas (SdH) oscillations starting from around 3T. We also analyse the angle and temperature dependence of these oscillations.

TT 21.4 Mon 16:30 H51

VOTCA-STP - Multi Scale Modeling of Spin Transport in Organic Semiconductors — •Erik R. McNellis, Shayan Hematiyan, Amaury Melo Souza, Sebastian Müller, and Jairo Sinova — Johannes Gutenberg University, Mainz, Germany

Organic molecules present a range of unique and highly attractive properties in solid state technology applications. So also in spintronics, where the weak but highly tailorable spin-orbit coupling in light elements offers spin lifetimes of unparalleled length and controllability.

1st-principles theoretical modeling stands to provide a crucial perspective on the emerging field of spin transport in organic semiconductors. Comprehensive modeling of relevant systems is challenging, with several of the spin transport mechanisms in traditional solid state materials non-existent or strongly modified in organics.

We are developing a multi-scale modeling framework for spin transport in bulk organic materials, based on the VOTCA toolkit for charge transport in the same. The core component is a semi-classical kinetic Monte-Carlo model, with input parameters calculated using 1st-principles theory.

The scope, capabilities of and particular challenges for this development will be presented along with possible extensions to e.g. 'spinterfaces', where spin currents are manipulated by tailoring of an inorganic / organic solid interface, as well as a perspective on the potential ramifications for experimental work in the field.

15 min. coffee break

TT 21.5 Mon 17:00 H51

High-pressure and nonlinear elastic response of solids: Example of carbon allotropes — •Pasquale Pavone, Rostam Golesorkhtabar, Stefan Kontur, and Claudia Draxl — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin, Germany

As prototype materials showing strong nonlinear elastic behaviour, diamond and, more recently, layered carbon allotropes have attracted much attention. However, even the nonlinear elasticity of diamond is not completely clarified: Experimentally, nonlinear elastic constants of diamond were investigated only recently [1], showing significant discrepancies with theoretical results. Furthermore, the standard ab-initio reference calculation for diamond [2] is nowadays about 30 years old and needs to be updated in the light of current development of theory, numerical algorithms, and available computer power. Using the full-potential all-electron package `exciting` [3], we perform a systematic ab-initio investigation of the nonlinear elastic properties of diamond, graphene monolayers, as well as simple-hexagonal and hexagonal graphite. We develope an extension of the `ElaStic` tool [4] for the determination of third-order elastic constants. From these results the pressure dependence of linear elastic constants is obtained and connected to dynamical quantities like the mode Grüneisen parameters.

[1] J.M. Lang *et al.*, Phys. Rev. Lett. **106**, 125502 (2011).
[2] O.H. Nielsen, Phys. Rev. B **34**, 5808 (1986).
[3] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[4] R. Golesorkhtabar *et al.*, Comp. Phys. Commun. **184**, 1861 (2013).

TT 21.6 Mon 17:15 H51

Calculations of temperature dependent resistivity for transition metals from the first principles — •David Wagenknecht[1,2], Ilja Turek[1,2], and Karel Carva[1] — [1]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University in Prague; Ke Karlovu 3, 12116 Prague 2, Czech Republic — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic; Žižkova 22, 61662 Brno, Czech Republic

The temperature dependence of electrical resistivity is studied from the first principles. Properties of late transition metals have been calculated using the linear muffin-tin orbital (LMTO) method with the coherent potential approximation (CPA). The influence of non-zero temperature has been described by a frozen lattice disorder – atoms were moved from the positions on an ideal lattice and different temperatures are then given by the magnitudes of the random displacement vectors. Dependence of the physical quantities on the parameters of the displacements (like random and non-random directions of the displacement vectors) has been observed and taken into account during discussion of the results. Special attention has been paid to an influence of spin-orbit interaction on the final resistivity, as well as to comparison with other *ab initio* calculations and experimental data; the obtained results agree reasonably well with those of other authors. Derived analytical modifications of the LMTO potential functions and the numerical codes can be now used to calculate relevant physical properties of different materials.

TT 21.7 Mon 17:30 H51

Ab Initio Molecular Dynamics Study of Conjugated Polymer Systems: The Elusive Localization of the Polaron — •Håkan W. Hugosson[1], Amina Mirsakiyeva[1], and Anna Delin[1,2] — [1]Department of Materials och Nano Physics, KTH Royal Institute of Technology, Stockholm, Sweden. — [2]Ångstrom Laboratory, Uppsala University, Uppsala, Sweden.

The thermoelectric conjugated polymer poly(3,4-ethylenedioxythiophene), or PEDOT, contains a carbon backbone consisting of alternating short and long carbon bonds. Therefore there are two isomeric states: aro-

matic and quinoid. Charge injection or the presence of charged doping agents leads to the formation of localized charge in the conjugated polymer - a so-called polaron. This polaron induces a localized structural distortion (a shift from the aromatic form towards the quinoid) in the conjugated carbon backbone.

Self-localized polarons in conjugated carbon systems have been found using semi-empirical or HF-theory, but formerly never using DFT with local or gradient corrected functionals (e.g. LDA/BLYP). Self-localization has been seen using DFT and long range hybrid functionals with partial exact exchange included.

Using modern ab initio molecular dynamics methods based on DFT we have studied PEDOT and its charge carrying polarons. A localized polaron is now found when studying the time-averaged changes in bond-distances and also in snap-shots for the frontier orbitals for long oligomers (12 monomers).

TT 22: Graphene: Fabrication (Joint session of DS, DY, HL, MA, O and TT organized by HL)

Time: Monday 17:45–18:45 Location: H17

TT 22.1 Mon 17:45 H17

Growth and characterization of mono- and bilayer graphene nanoribbons grown on SiC(0001) — •Lauren Aranha Galves, Joseph Wofford, Uwe Jahn, João Marcelo J. Lopes, and Henning Riechert — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

Graphene Nanoribbons (GNRs) are promising for applications in nanoelectronics due to their unique properties. Unlike graphene sheets, GNRs possess a bandgap and the gap is inversely proportional to their width [1]. Additionally, bilayer GNRs offer the possibility to further tune their bandgap via the application of an external electric field [2]. The thermal decomposition of SiC surfaces is a suitable synthesis method for GNRs due to the control it offers over their size [3].

In this report we present the structural characterization of mono- and bilayer GNRs grown on SiC(0001) by surface graphitization. Bilayer GNRs were obtained via a post-growth air-annealing process [4]. The width of the ribbons were determined via atomic force microscopy (AFM) height and phase imaging as well as scanning electron microscopy (SEM), while the number of layers (i.e. mono or bilayer GNRs) were examined by Raman spectroscopy. Based on these measurements it was possible to identify an activation energy for the formation of the nanostructures and a lateral etching effect in the bilayer GNRs due to the air-annealing process.

[1] Barone et al., Nano Lett. 6, 2748 (2006); [2] Li et al., Eur. Phys. J. 64, 73 (2008); [3] Sprinkle et al. Nat. Nanotechnol. 5, 727 (2010); [4] Oliveira Jr. et al., Nat. Comm. 6, 7632 (2015).

TT 22.2 Mon 18:00 H17

Optoelectronic Properties of Graphene Nano-Ribbons Patterned By Helium Ion Beam Lithography — •Akshay Kumar Mahadev Arabhavi[1], Andreas Brenneis[1,2], Simon Drieschner[1,2], Marcus Altzschner[1], Helmut Karl[3], Jose Garrido[1,2], and Alexander Holleitner[1,2] — [1]Walter Schottky Institut and Physics-Department, Technical University Munich, Am Coulombwall 4a, 85748 Garching, Germany. — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 Munich, Germany. — [3]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany.

High electron mobility, excellent thermal conductivity and uniform absorption in the visible range makes graphene an outstanding material for high-frequency optoelectronic applications. However, the lack of a band gap limits graphene in switching applications. A quantization energy can be introduced by confining graphene to one-dimensional ribbons of widths below 20 nm, for instance, using Helium Ion Beam Lithography (HIBL) [1-2]. We have optimized the parameters to pattern graphene nano-ribbons on sapphire substrates using HIBL, such as dose, beam current, spot control and dwell time. Moreover, we apply an ultrafast photocurrent spectroscopy [3] to investigate the optoelectronic properties of the patterned graphene nano-ribbons with respect to their high-frequency properties. References: [1] M. Han et al., Phys. Rev. Lett. 98, 206805, (2007). [2] Bell DC et al., Nanotechnology 20, 455301, (2009). [3] A. Brenneis, et al., Nature Nanotech, 10, 135, (2015).

TT 22.3 Mon 18:15 H17

High quality bilayer graphene from chemical vapor deposition on reusable copper — •Michael Schmitz[1], Stephan Engels[1,2], Luca Banszerus[1], Kenji Watanabe[3], Takashi Taniguchi[3], Bernd Beschoten[1], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

We recently introduced a dry transfer method for single-layer graphene grown by chemical vapor deposition (CVD) yielding ultra high quality graphene comparable to the best exfoliated samples [1]. Here, we demonstrate that this method can be extended to bilayer graphene. In particular, we show the fabrication and characterization of bilayer graphene/hexagonal boron nitride heterostructures using high quality CVD bilayer graphene grown on reusable copper foils. Raman measurements reveal a high structural quality [2]. We achieve carrier mobilities up to 45,000 $cm^2/(Vs)$ at 1.8 K and up to 17,000 $cm^2/(Vs)$ at room temperature outperforming all state-of-the-art CVD bilayer graphene devices. Finally, we show dual-gated transport measurements to investigate band-gap opening in our CVD grown bilayer graphene.

[1] L. Banszerus, M. Schmitz, S. Engels *et al.*, Science Advances **1**, e1500222 (2015)
[2] C. Neumann, S. Reichardt, P. Venezuela *et al.*, Nature Communications **6**, 8429 (2015)

TT 22.4 Mon 18:30 H17

Graphene-based fast hot-electron bolometer with bandwidth from THz to VIS — Martin Mittendorff[1,2], Josef Kamann[3], Jonathan Eroms[3], Dieter Weiss[3], Christoph Drexler[3], Sergey D. Ganichev[3], Jochen Kerbusch[2], Artur Erbe[2], Ryan J. Suess[1], Thomas E. Murphy[1], Jacob C. König-Otto[2,4], Harald Schneider[2], Manfred Helm[2,4], and •Stephan Winnerl[2] — [1]University of Maryland, College Park, USA — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Universität Regensburg, Regensburg, Germany — [4]Technische Universität Dresden, Dresden, Germany

We present a fast detector (rise time 40 ps) operating at room temperature that is capable to detect radiation from the THz to visible spectral range (demonstrated wavelengths 500 μm - 780 nm) [1]. The detector consists of a CVD-grown graphene flake contacted by a broadband logarithmic periodic antenna. SiC acts as a substrate material that does not interfere with the detection mechanism in the desired frequency range, even within the Reststrahlen band of SiC (6 - 12 μm). The detector is ideal for timing purposes. Near infrared (mid- and far infrared) pulse energies of the order of 10 pJ (1 nJ) are sufficient to obtain good signal-to-noise ratios. We suggest that the bandwidth is limited by the antenna dimensions (typically several mm) on the long wavelength side and by the bandgap of SiC (380 nm) on the short wavelength side.

[1] M. Mittendorff et al., Opt. Express 23, 28728 (2015).

TT 23: Quantum Information Systems (Joint session of HL, MA, O and TT organized by HL)

Time: Tuesday 9:30–12:30 Location: H15

TT 23.1 Tue 9:30 H15

Nuclear spins as quantum memories for quantum networks and repeaters — •Andreas Reiserer[1,2], Norbert Kalb[1,2], Machiel Blok[1,2], Koen van Bemmelen[1,2], Tim Taminiau[1,2], and Ronald Hanson[1,2] — [1]Kavli Institute of Nanoscience, TU Delft, The Netherlands — [2]QuTech, TU Delft, The Netherlands

A future quantum network will consist of quantum processors that are connected by quantum channels, just like conventional computers are wired up to form the Internet. To realize such network, we plan to use spin qubits in diamond, which combine access to few-qubit nuclear-spin registers with exceptional coherence properties. However, preserving the coherence of the register while generating entanglement between remote spins is an open challenge.

Here, we investigate the coherence of single ^{13}C spins that occur in an otherwise spin-free diamond sample of natural isotope abundance. Five individual nuclear spins are controlled via the weak hyperfine interaction with the electronic spin of a nitrogen vacancy (NV) center in a strong magnetic field. We encode quantum bits in the nuclear spins and investigate the loss of coherence caused by repeated electron spin initialization, which is required for any quantum protocol that is subject to errors. Encoding the qubits in a decoherence-protected subspace of two rather than one nuclear spin increases the robustness of the protocol and enables the investigation of a large parameter space with a single sample. Our results open perspectives for the realization of large scale quantum networks and quantum repeaters using NV centers with weakly coupled nuclear spins.

TT 23.2 Tue 9:45 H15

Long distance coupling of resonant exchange qubits — •Maximilian Russ and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We investigate the effectiveness of a microwave cavity as a mediator of interactions between two resonant exchange (RX) qubits [1,2] in semiconductor quantum dots (QDs) over long distances [3], limited only by the extension of the cavity. Our interaction model includes the orthonormalized Wannier orbitals constructed from Fock-Darwin states under the assumption of a harmonic QD confinement potential. We calculate the qubit-cavity coupling strength g_r in a Jaynes Cummings Hamiltonian, and find that dipole transitions between two states with an asymmetric charge configuration constitute the relevant RX qubit-cavity coupling mechanism. The effective coupling between two RX qubits in a shared cavity yields a universal two-qubit iSWAP-gate with gate times on the order of nanoseconds over distances on the order of up to a millimeter.

[1] J. Medford et al., Phys. Rev. Lett. **111**, 050501 (2013).
[2] J. M. Taylor, V. Srinivasa, and J. Medford, Phys. Rev. Lett. **111**, 050502 (2013).
[3] M. Russ and G. Burkard, arXiv: 1508.07122 (2015)

TT 23.3 Tue 10:00 H15

Higher Order Spin Correlation in Semi-Conductor Quantum Dots — •Nina Fröhling, Jan Böker, and Frithjof Anders — Fakultät Physik, TU Dortmund, 44227 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. In a mean field approach the nuclear spin field is assumed to be frozen, since the precession frequency of the electron in the nuclear hyperfine field is much greater than the precession frequency of the nuclei in the hyperfine field of the electron. Since the higher order cumulants of this mean-field approximation vanish, these functions can serve as a tool to reveal the entanglement between the electron spin and the nuclear spin bath. We also evaluate analytically the symmetries exhibited by third order correlation functions in the high-temperature limit. It can be shown that the third order correlation function is constrained to a small subspace of all possible frequencies. Furthermore, we calculate the third order correlation function using the Lanczos-algorithm and statistic trace evaluation. The viability of this method is benchmarked by the analysis of the established spin noise spectrum given by the second order correlation function.

TT 23.4 Tue 10:15 H15

Spin Decoherence in a Pulsed Quantum Dot System — •Natalie Jäschke and Frithjof Anders — Fakultät Physik, TU Dortmund, 44227 Dortmund, Deutschland

In pump-probe experiments electron spin polarization in a semiconductor quantum dot is generated by periodic optical excitations. The decoherence of this polarization is dominated by the hyperfine interaction with a bath of nuclear spins in the short time regime. We aim for a theory that combines the effect of the periodic laser 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 Overhauserfield bridges the time until the next laser pulse. We analyze the stability of different non-equilibrium nuclear spin bath distribution functions as well as the magnetic field dependent build up of a laser-induced nuclear spin polarization.

TT 23.5 Tue 10:30 H15

A model for slow decoherence in semiconductor quantum dots — •Wouter Beugeling, Frithjof B. Anders, and Götz S. Uhrig — Lehrstuhl für Theoretische Physik I/II, Technische Universität Dortmund, 44221 Dortmund, Germany

Quantum dots on semiconductor materials have been proposed as candidates for quantum computational applications. The information is carried by a single electron spin, which interacts with the substrate nuclei with a hyperfine coupling. The electron spin is manipulated with excitation by periodic laser pulses and by an external magnetic field. The nuclear spins can be polarized indirectly, due to the hyperfine coupling, an effect known as dynamical nuclear polarization.

The leading contribution in the dynamics is the Larmor precession, which dephases due to small frequency shifts from the hyperfine coupling. Typically, the dephasing causes almost complete decoherence at the time scale of the pulse interval. Thus, a different mechanism must be responsible for the finite coherence observed in experiments.

In this presentation, we propose a mechanism explaining the experimental findings. We study the dynamics using the Lindblad equation, which includes the non-unitarity from the decay of the excited state. We separate the time scales of the Larmor precession (fast) and the nuclear-spin dynamics (slow) by treating the hyperfine couplings in a perturbative fashion. We find low-frequency contributions that dephase at a much slower rate, providing a plausible explanation for the finite coherence at the pulse interval time. We support this claim with analytical derivations and numerical results.

30 min. Coffee Break

TT 23.6 Tue 11:15 H15

Force sensing via individual nitrogen-vacancy spins in diamond mechanical resonator — Phani Peddibhotla[1], Michael Barson[2], Kumar Ganesan[3], Preeti Ovartchaiyapong[5], Berndt Koslowski[4], Ania Jayich[5], Steven Prawer[3], Neil Manson[2], Marcus Doherty[2], and •Fedor Jelezko[1] — [1]Institute for Quantum Optics, University of Ulm, 89081 Ulm, Germany — [2]Laser Physics Centre, Australian National University, Canberra, Australia — [3]School of Physics, University of Melbourne, Victoria 3100, Australia — [4]Institute for Solid State Physics, University of Ulm, 89081 Ulm, Germany — [5]Department of Physics University of California, Santa Barbara

We propose to use the embedded nitrogen-vacancy (NV) defect states in single-crystal diamond cantilever for measuring external forces. In order to experimentally demonstrate the force sensing capabilities, we employed an atomic force microscope (AFM) tip to apply a force on the non-clamped end of the diamond cantilever, which in turn induces lattice strain to a NV center close to the clamping point of a cantilever. The strain-mediated coupling between NV spin and diamond mechanics is observable via clear signatures in the optically detected electron spin resonance (ESR) spectrum of the NV center [1, 2].

[1] J. Teissier et al., PRL 113, 020503 (2014). [2] P. Ovartchaiyapong,

et al., Nat. Commun. 5:4429 (2014).

TT 23.7 Tue 11:30 H15

Identification of the positively charge Nitrogen Vacancy center in diamond — Helmut Fedder[1], •Sina Burk[1], Mathias Pfender[1], Nabeel Aslam[1], Sebastian Zaiser[1], Philipp Neumann[1], Andrej Denisenko[1], Patrick Simon[2], José Garrido[2], Martin Stutzmann[2], Marcus Doherty[3], Neil Manson[3], Audrius Alkauskas[4], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Uni Stuttgart — [2]Walter Schottky Institut, TU München — [3]Australian National University, Canberra, Australia — [4]Center for Physical Sciences and Technology, Lithuania

Electron and nuclear spins associated with point defects in semiconductors are promising systems for solid state quantum technologies with applications in quantum information processing and quantum sensing. In a typical quantum register architecture, an electron spin is used as an ancilla for readout and control, whereas nuclear spins serve as register qubits [1-2]. Flip-flop processes of the electron spin limit the nuclear spin coherence time. This limitation can be overcome by controlling the defect's ionization state. Here we increase the coherence time of the ^{14}N nuclear spin associated with the Nitrogen-Vacancy center in diamond by controlling its charge state. We exploit planar double junction diodes fabricated by surface transfer doping with hydrogen [3] to rapidly switch the charge state from NV^- (S=1) to NV^+ (S=0). We verify the NV^+ state by nuclear magnetic resonance and demonstrate the enhancement of the ^{14}N coherence time. [1] Saeedi et al., Science 342, 830 (2013). [2] P.C. Maurer et al., Science 336, 1283 (2012). [3] M. Hauf et al., Nano Lett. 14, 2359 (2014)

TT 23.8 Tue 11:45 H15

Electrical Charge State Control of Single Defects in Silicon Carbide — •Matthias Widmann[1], Sang-Yun Lee[1], Matthias Niethammer[1], Ian Booker[2], Takeshi Ohshima[3], Nguyen Tien-Son[2], Adam Gali[4], Erik Janzén[2], and Jörg Wrachtrup[1] — [1]3.Phys. Institut, Stuttgart — [2]Dep. of Phys., Linköping — [3]Japan AEA, Takasaki — [4]Wigner Res.C f.Phys., Budapest

Atomic scale defects in solids attracted a lot of interest over the last decade, because their spins can be used to detect magnetic- and electric fields and temperature with high sensitivity. They are also promising candidates as qubits and used for quantum information processing. Mostly color centers in diamond, e.g. NV centers, and impurities in silicon are used in the past. A single NV spin can be read out optically at room temperature. Electrical readout is possible, but remains challenging. Spins in silicon can be driven and read out electrically very well, however require low temperatures. Spins in silicon carbide (SiC) can overcome these drawbacks. Their spins can be driven and detected both optically[1] and electrically at ambient conditions. SiC electrical properties are promising since integrated single spins in modern electronic devices will allow manipulation of spins in various manners. Here we extend our single defect studies[1] towards electrical manipulation of its charge state in order to get better insight about creation of isolated defects with desired spin quantum number. We will also present how the charge state control affects spin control, and discuss possible applications. 1. M. Widmann et al.,Nat. Mat. 14 (2015)

TT 23.9 Tue 12:00 H15

Spin Coherence Time of Si Vacancies in Silicon Carbide Exceeding One Millisecond — •D. Simin[1], H. Kraus[1,2], A. Sperlich[1], T. Ohshima[2], G. V. Astakhov[1], and V. Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Wuerzburg, 97074 Wuerzburg — [2]Japan Atomic Energy Agency (JAEA), 370-1292 Takasaki, Japan — [3]ZAE Bayern, 97074 Wuerzburg

Quantum information processing has been the hot topic in the field of information theory for several decades. While great progress was achieved, both on the theoretical and experimental field, to recognize and to employ the most suitable material and information carrier from the vast amount of possibilities is still the main goal of ongoing research activities all over the world. Whereas a wide availability and easy handling are crucial for a functioning device, long-preserving spin coherence is also essential for such a system. Therefore, we investigate the coherence time properties of the Si-vacancies in a 4H-SiC wafer using the pulsed-ODMR technique. Implementing the common Rabi-, Ramsey-, Spin-Echo- and CPMG-sequences, we can precisely measure spin-lattice (T_1) and spin-spin (T_2) relaxation times. The measurements are not only conducted at ambient conditions, but also at different temperatures and in different magnetic fields. In particular, the coherent spin properties of the V_{Si} defect are investigated in the temperature range from 10K to 300K and at magnetic field strengths of up to 30mT. Using dynamic decoupling protocols we achieve spin coherence time exceeding 1ms, demonstrating the high potential of SiC for various quantum applications.

TT 23.10 Tue 12:15 H15

Controlled Implantation of Silicon Vacancy Layers for Quantum Applications in Bulk Silicon Carbide — •H. Kraus[1,2], C. Kasper[2], S.-I. Sato[1], M. Haruyama[1], S. Onoda[1], T. Makino[1], T. Ohshima[1], G. Astakhov[2], and V. Dyakonov[2,3] — [1]Japan Atomic Energy Agency, Takasaki, Gunma, Japan — [2]Exp. Physics VI, Julius Maximilian University of Würzburg — [3]ZAE Bayern, Würzburg

Quantum centers in silicon carbide (SiC) have already transcended their former reputation as mere performance-hampering defects. Their long spin lifetime, unique spin-preserving optical pumping mechanism[1], and the possibility of downscaling to single-photon source level[2,3] makes them viable candidates for a plethora of quantum applications in sensing, rf devices, and quantum computing.

One quantum center species, the silicon vacancy (V_{Si}), can be reliably and homogeneously produced in the bulk by electron or neutron[3] irradiation. In contrast, a method to implant defects at a specific depth would be very interesting, especially when aiming for spatially separated centers for single photon sources. We present a study on proton irradiation to create a layer of V_{Si} in an irradiation-energy-tunable depth in bulk SiC. We discuss the spectroscopic response of this layer, and compare the V_{Si} depth profile—measured by confocal microscopy—with the H^+ stopping power of silicon carbide. Finally, we extend this study on the effects of high energy heavy ion damage.

[1] H. Kraus et al., Nature Phys. **10**, 157 (2014)
[2] M. Widmann et al., Nature Mater. **14**, 164 (2015)
[3] F. Fuchs et al., Nature Commun. **6**, 7578 (2015)

TT 24: Transport: Weyl Semimetals

Time: Tuesday 9:30–13:00 Location: H18

Invited Talk TT 24.1 Tue 9:30 H18

Detecting Weyl fermions in condensed matter — •Titus Neupert — Princeton Center for Theoretical Science, Princeton University, Princeton, New Jersey 08544, USA

Weyl semimetals are three-dimensional materials with topologically protected degeneracy points in the band structure. Even though this material class was envisioned several decades ago and anticipated in many theoretical studies, it took until the beginning of this year to find the first Weyl semimetal TaAs. In this talk, I will give an overview over the characteristic properties of Weyl semimetals, and more broadly three-dimensional topological semimetals. I will then discuss recent experiments that probe the physics of Weyl semimetals. For example, angle resolved photoemission spectroscopy measurements evidence the topological surface states, so-called Fermi arcs. Magnetotransport measurements detect a characteristic negative magnetoresistance associated with a nonconservation of the chiral charge of excitations near the Weyl points. This effect has a beautiful correspondence to the chiral anomaly studied in high-energy physics.

TT 24.2 Tue 10:00 H18

ARPES study of possible new Weyl semimetals — •Erik Haubold[1], Yevhen Kushnirenko[1], Alexander Fedorov[1], Seunghyun Khim[1], Sabine Wurmehl[1,2], Dmitriy Efremov[1], Timur Kim[3], Moritz Hoersch[3], Bernd Büchner[1,2], and Sergey Borisenko[1] — [1]IFW Dresden, Institut für Festkörperforschung, Postfach 270116, 01171 Dresden — [2]Institut für Festkörperphysik, TU Dresden, 01062 Dresden — [3]Diamond Light Source, Harwell Campus, Didcot OX11 0DE, United Kingdom

Development of modern electronics struggles with the ongoing decrease of the structural size. New approaches, for example spintronic devices, could solve these problems as they utilize intrinsic properties of the

materials like the spin. The most promising materials for these applications are topological insulators and (Weyl-) semimetals as they possess unique surface and bulk properties which could enable direct spin manipulation. The goal of this contribution is to find new materials belonging to the group of Weyl semimetals. Weyl semimetals host the electrons which behave as Weyl Fermions — non-degenerate versions of Dirac fermions. To check for the presence of these states we use angle-resolved photoemission spectroscopy at synchrotrons, as it directly resolves the 3D electronic structure of the materials and therefore gives direct insight into their electronic structure. One of the materials to be studied is $TaIrTe_4$, which is a similar compound to the already proposed WTe_2. This choice is supported by band structure calculations indicating the possible presence of Weyl fermions in this compound.

TT 24.3 Tue 10:15 H18

Anisotropic density fluctuations, plasmons, and Friedel oscillations in nodal line semimetal — •Jun Won Rhim[1] and Yong Baek Kim[2] — [1]Max-Planck Institute for the Physics of Complex Systems — [2]Department of Physics and Center for Quantum Materials, University of Toronto, Toronto, Ontario M5S 1A7, Canada

Motivated by recent experimental efforts on three-dimensional semimetals, we investigate the static and dynamic density response of the nodal line semimetal by computing the polarizability for both undoped and doped cases. The nodal line semimetal in the absence of doping is characterized by a ring-shape zero energy contour in momentum space, which may be considered as a collection of Dirac points. In the doped case, the Fermi surface has a torus shape and two independent processes of the momentum transfer contribute to the singular features of the polarizability even though we only have a single Fermi surface. In the static limit, there exist two independent singularities in the second derivative of the static polarizability. This results in the highly anisotropic Friedel oscillations which show the angle-dependent algebraic power law and the beat phenomena in the oscillatory electron density near a charged impurity. Furthermore, the dynamical polarizability has two singular lines along $\hbar\omega = \gamma p$ and $\hbar\omega = \gamma p \sin\eta$, where η is the angle between the external momentum $\vec{p}$ and the plane where the nodal ring lies. From the dynamical polarizability, we obtain the plasmon modes in the doped case, which show anisotropic dispersions and angle-dependent plasma frequencies.

TT 24.4 Tue 10:30 H18

Superconductivity in Weyl Semimetal Candidate $MoTe_2$ — •Yanpeng Qi[1], Pavel Naumov[1], Mazhar Ali[2], Catherine Rajamathi[1], Oleg Barkalov[1], Michael Hanfland[3], Shu-Chun Wu[1], Chandra Shekhar[1], Yan Sun[1], Vicky Süss[1], Marcus Schmidt[1], Ulrich Schwarz[1], Eckhard Pippel[4], Peter Werner[4], Reinald Hillebrand[4], Tobias Förster[5], Erik Kampert[5], Walter Schnelle[1], Stuart Parkin[4], Robert Cava[2], Claudia Felser[1], Binghai Yan[1,6], and Sergey Medvedev[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Chemistry, Princeton University, Princeton, USA — [3]European Synchrotron Radiation Facility, Grenoble, France — [4]Max Planck Institute of Microstructure Physics,Halle, Germany — [5]Dresden High Magnetic Field Laboratory,Dresden, Germany — [6]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

In this work, we investigate the sister compound of WTe_2, $MoTe_2$, which is also predicted to be a Weyl semimetal and a quantum spin Hall insulator in bulk and monolayer form, respectively. We find that $MoTe_2$ exhibits superconductivity with a resistive transition temperature T_c of 0.1 K. The application of a small pressure is shown to dramatically enhance the T_c, with a maximum value of 8.2 K being obtained at 11.7 GPa (a more than 80-fold increase in Tc). This yields a dome-shaped superconducting phase diagram. Further explorations into the nature of the superconductivity in this system may provide insights into the interplay between superconductivity and topological physics.

TT 24.5 Tue 10:45 H18

Bulk Fermi Surface Topology of the Weyl Semimetal Tantalumarsenide — •Marcel Naumann[1], Frank Arnold[1], Shu-Chun Wu[1], Yan Sun[1], Marcus Peter Schmidt[1], Horst Borrmann[1], Claudia Felser[1], Binghai Yan[1,2], and Elena Hassinger[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Max Planck Institute for Physics of Complex Systems, 01187 Dresden, Germany

Tantalumarsenide is a member of the non-centrosymmetric monopnictides which are putative Weyl semimetals. We have reconstructed the Fermi surface topology of TaAs by angular dependent Shubnikov-de Haas and de Haas-van Alphen measurements of a high quality single crystal and ab initio density-functional theory bandstructure calculations. By fitting the experimental angular dependence of the quantum oscillation frequencies to the calculated DFT bandstructure, we were able to reconstruct the entire Fermi surface and identify individual electron and hole pocket orbits in our measurements. We find that the Fermi surface consists of eight distinct pockets along each nodal ring, three pairs of topologically non-trivial electron Weyl-pockets and two trivial hole-pockets. Their effective charge carrier masses and scattering times have been determined by temperature and magnetic field dependencies of the quantum oscillation amplitude. Unlike the other members of the non-centrosymmetric monopnictides, TaAs is the first Weyl metal candidate were the Fermi energy is sufficiently close to both Weyl points to generate separate Weyl pockets with different chiralities.

TT 24.6 Tue 11:00 H18

Low energy electronic scattering processes in the topological Weyl semimetal TaAs — •Silvia Müllner[1], Peter Lemmens[1], Vladimir Gnezdilov[1,2], Raman Sankar[3], and Fangcheng Chou[3] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE NAS, Ukraine — [3]CCMS, National Taiwan Univ., Taipei, Taiwan

The topological Weyl semimetal TaAs shows Weyl points as well as topological surface states (Fermi arcs) intimately related to symmetry and strong spin orbit interaction. We find evidence for a low energy maximum in the scattering intensity that is compatible with electronic correlations in a collision dominated regime. We compare our observations with topological insulators.

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

15 min. break

TT 24.7 Tue 11:30 H18

Apparent negative magnetoresistance without independent Weyl pockets in the Weyl semimetal TaP — •Elena Hassinger[1], Frank Arnold[1], Marcel Naumann[1], Shu-Chun Wu[1], Yan Sun[1], Ricardo Donizeth dos Reis[1], Mukkattu O. Ajeesh[1], Chandra Shekhar[1], Nitesh Kumar[1], Marcus Schmidt[1], Adolfo Grushin[2], Jens Bardarson[2], Michael Baenitz[1], Horst Borrmann[1], Michael Nicklas[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Max Planck Institute for Physics of Complex Systems, Dresden, Germany

In the recently discovered Weyl semimetals, an unconventional negative longitudinal magnetoresistance is expected due to a phenomenon called chiral anomaly. An open question is, how close the Fermi energy needs to be to the Weyl nodes, in order to detect this phenomenon. This question can only be adressed by knowing the electronic bandstructure, i.e. the position of the Fermi energy, and the intrinsic longitudinal magnetoresistance precisely. Here, we report the detailed Fermi surface topology of the Weyl semimetal TaP determined via angle-resolved quantum oscillation spectra combined with bandstructure calculations. The Fermi surface consists of an electron and a hole banana without independent pockets around the Weyl points. Although the absence of independent Fermi surface pockets around the Weyl points means that no chiral anomaly is expected, we detect a negative longitudinal magnetoresistance. We discuss possible origins.

TT 24.8 Tue 11:45 H18

Magnetic resonance as a local probe for linear bands in the Weyl semimetals NbP and TaP — •Michael Baenitz, Hiroshi Yasuoka, Mayukh Majumder, Chandra Shekhar, Binghai Yan, Claudia Felser, and Markus Schmidt — MPI for Chemical Physics of Solids, 01187 Dresden, Germany

Some compensated d-electron semimetals, for example the monophosphites NbP and TaP, with non centrosymmetric structure and with sizable spin orbit coupling (SOC) form a new class of material: the Weyl semimetals (WSM). A unique linear crossing of valence- and conduction- band in a single point in reciprocal space defines the so called Weyl point where the fermion mass vanishes theoretically. In real materials the Fermi level E_F does not exactly match the Weyl

node and as a consequence residual very light fermions are found. Due to the SOC these Weyl fermions have a chirality (handedness) on their linear dispersive ($E \propto k$) bands and frequently a linear density of states (DOS) at the Fermi level E_F. We use NMR as a probe for this linear d-electron bands. The shift provides the s- and d- electron contributions to the DOS at E_F, whereas the spin lattice relaxation is governed by low energy excitations around E_F. ^{31}P (I = 1/2) - Fourier - transform - and ^{95}Nb (I = 9/2) - broadline - sweep - NMR studies are performed. We investigated powder samples as well as single crystals on both systems. The angular dependence of the ^{95}Nb- and ^{31}P - NMR lines is discussed.

TT 24.9 Tue 12:00 H18

Fermi-surface topology of the Weyl semimetal NbP — •J. Klotz[1,2], Shu-Chun Wu[3], Chandra Shekhar[3], Yan Sun[3], Marcus Schmidt[3], Michael Nicklas[3], Michael Baenitz[3], M. Uhlarz[1], J. Wosnitza[1,2], Claudia Felser[3], and Binghai Yan[3,4] — [1]Hochfeld-Magnetlabor (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The recent discovery of Weyl semimetals in transition-metal monopnictides revealed an exotic topological matter. Weyl semimetals feature band crossings with massless dispersions in their bulk band structure, termed Weyl points. Here, we present a Fermi-surface study on the Weyl semimetal NbP that combines both experimental data and band-structure calculations. We employed torque magnetometry in order to measure the angular dependence of the de Haas-van Alphen effect in a 12 T / 350 mK system. The excellent agreement between measured and calculated quantum-oscillation frequencies evidences the existence of two electron and two hole pockets and allows to locate the position of the Weyl points with respect to the Fermi energy.

TT 24.10 Tue 12:15 H18

Visualizing the chiral anomaly in Dirac and Weyl semimetals with photoemissspectroscopy — •Jan Behrends[1], Adolfo G Grushin[3], Teemu Ojanen[2], and Jens H Bardarson[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Low Temperature Laboratory, Department of Applied Physics, Aalto University, FI-00076 AALTO, Finland — [3]Department of Physics, University of California, Berkeley, CA 94720, USA

Quantum anomalies are the breaking of a classical symmetry by quantum fluctuations. They dictate how physical systems of diverse nature, ranging from fundamental particles to crystalline materials, respond topologically to external perturbations, insensitive to local details. In the solid state, it fundamentally affects the properties of topological Weyl and Dirac semimetals, recently realized experimentally.

In this work we propose that the most identifying consequence of the chiral anomaly, the charge density imbalance between fermions of different chirality induced by non-orthogonal electric and magnetic fields, can be directly observed in these materials with the existing technology of photoemission spectroscopy. With angle resolution, the chiral anomaly is identified by a characteristic note-shaped pattern of the emission spectra, originating from the imbalanced occupation of the bulk states and a previously unreported momentum dependent energy shift of the surface state Fermi arcs. Thereby, our work provides essential theoretical input to foster the direct visualization of the chiral anomaly in condensed matter.

TT 24.11 Tue 12:30 H18

Unconventional superconductivity in YPtBi and related topological semimetals — •Markus Meinert — Center for Spinelectronic Materials and Devices, Bielefeld University, Germany

YPtBi, a topological semimetal with very low carrier density, was recently found to be superconducting below $T_c = 0.77$ K. In the conventional theory, the nearly vanishing density of states around the Fermi level would imply a vanishing electron-phonon coupling and would therefore not allow for superconductivity. Based on relativistic density functional theory calculations of the electron-phonon coupling in YPtBi it is found that carrier concentrations of more than 10^{21} cm^{-3} are required to explain the observed critical temperature with the conventional pairing mechanism, which is several orders of magnitude larger than experimentally observed. It is very likely that an unconventional pairing mechanism is responsible for the superconductivity in YPtBi and related topological semimetals with the Half-Heusler structure.

TT 24.12 Tue 12:45 H18

Three-dimensional Dirac semimetal films grown by molecular beam epitaxy — Debakanta Samal[1], •Hiroyuki Nakamura[1], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Stuttgart, Germany — [3]Department of Physics, University of Tokyo, Japan

Antiperovskite compounds have recently been predicted to host bulk three-dimensional Dirac dispersion as well as surface states protected by crystal symmetry. We present fabrication of cubic antiperovskite Sr_3PbO films, which has six Dirac points along high-symmetry momentum axes. Films were grown epitaxially on $LaAlO_3$ substrates by molecular beam epitaxy and capped with polymer to facilitate ex-situ transport characterization. All of the films showed metallic temperature dependence. The Hall effect measurement suggests that the carrier type is hole, with density between 10^{19} - 10^{20} cm^{-3}. We will describe our ongoing effort to tune the Fermi energy close to the Dirac point, as well as detail of the low temperature magnetotransport.

TT 25: Superconductivity: Fe-based Superconductors - 1111 & 111

Time: Tuesday 9:30–10:45 Location: H19

TT 25.1 Tue 9:30 H19

Crystal growth and characterization of *RE*FeAsO (*RE* = La, Nd) and LaFePO — •Agnes Adamski, Mahmoud Abdel-Hafiez, and Cornelius Krellner — Physikalisches Institut, Goethe Universität, D-60438 Frankfurt am Main

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 1111 systems, the focus has been rapidly shifted towards other materials, were large high-quality crystals are available. In contrast, the growth of sizeable high-quality single crystals of 1111 compounds is extremely challenging, slowing down the scientific progess in this type of compounds.

Here we report on the crystal growth of 1111-type materials under ambient pressure conditions and by using the flux technique. The influence of the material to flux ratio was systematically studied. Subsequently, the obtained samples were analyzed with powder diffractometry, electron microscope, energy dispersive x-ray analysis, Laue diffractometry and magnetic measurements to analyze the structural and magnetic properties.

TT 25.2 Tue 9:45 H19

Impact of concomitant Y and Mn substitution on properties of $La_{1-z}Y_zFe_{1-y}Mn_yAsO_{0.9}F_{0.1}$ — •Rhea Kappenberger[1,2], Franziska Hammerath[1,2], Mesfin Asfaw Afrassa[1,3], Pierre Rousse[1], Christian Hess[1], Giacomo Prando[1], Matteo Moroni[1], Samuele Sanna[4], Pietro Carretta[4], Gianrico Lamura[5], Anja U. B. Wolter[1], Sirko Kamusella[2], Hans-Henning Klauss[2], 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 — [3]Addis Ababa University, College of Natural Science, Addis Ababa, Ethiopia — [4]Dipartimento di Fisica and Unitá di CNISM di Pavia, Pavia, Italy — [5]CNR-SPIN and Universita di Genova, I-16146 Genova, Italy

The substitution of constituents is frequently used as a local probe to check the microscopic properties of an unconventional superconductor in response to such an "impurity".

In this talk, we present several structural parameters and the superconducting critical temperatures in response to different substitution levels of Mn and Y in $La_{1-z}Y_zFe_{1-y}Mn_yAsO_{0.9}F_{0.1}$. We will dis-

cuss our findings in the light of chemical pressure inflicted by Y, which has a significantly smaller ionic radius than La, and strong electron localization caused by small amounts of paramagnetic Mn impurities.

TT 25.3 Tue 10:00 H19

Unusual temperature evolution of superconductivity in LiFeAs — •Pranab Kumar Nag[1], Ronny Schlegel[1], Danny Baumann[1], Hans-Joachim Grafe[1], Robert Beck[1], Sabine Wurmehl[1,2], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

We have performed temperature dependent scanning tunneling spectroscopy on an impurity-free surface area of a LiFeAs single crystal [1]. Our data reveal a highly unusual temperature evolution of superconductivity: at $T_c^* = 18$ K a partial superconducting gap opens, as is evidenced by subtle, yet clear features in the tunneling spectra, i.e. particle-hole symmetric coherence peaks and dip-hump structures. At $T_c = 16$ K, these features substantiate dramatically and become characteristic of full superconductivity. Remarkably, this is accompanied by an almost jump-like increase of the gap energy at T_c to about 87% of its low-temperature gap value. The energy of the dip as measured by its distance to the coherence peak remains practically constant in the whole temperature regime $T \leq T_c^*$. We compare these findings with established experimental and theoretical results.
[1] P. K. Nag *et al.*, arXiv:1509.03431(2015)

TT 25.4 Tue 10:15 H19

Physical Properties of Off-Stoichiometric LiFeAs — •Uwe Gräfe[1], Shiv Jee Singh[1], Robert Beck[1], Hans-Joachim Grafe[1], Sabine Wurmehl[1,3], Christian Hess[1,2], and Bernd Büchner[1,3] — [1]IFW Dresden, Institut für Festkörperforschung, Postfach 270116 01171 Dresden — [2]Center for Transport and Devices, TU Dresden, 01169 Dresden — [3]Institut für Festkörperphysik, TU Dresden, 01062 Dresden

It is known that small modifications on the stoichiometry of LiFeAs have high impact on the physical properties in the normal and superconducting state. Here we present a systematic study on the Li-Fe-As system by XRD, NQR and resistivity. We synthesized samples with different nominal compositions of Li, Fe and As by solid state reaction and show that, besides stoichiometric LiFeAs, only enriching the system with Fe forms phase pure samples. The modifications due to this enrichment can be tracked by a shift of the NQR-frequency and the lattice constants. Thus NQR can be taken as a measure for the changes induced by additional Fe in Li-Fe-As. We further show that these changes are not only decreasing T_c but also cause a sudden reduction of normal state resistivity and electron-electron scattering. Altogether we therefore conclude that Fe has a charge doping effect on Li-Fe-As.

TT 25.5 Tue 10:30 H19

Superconductivity in LiFeAs probed with quasiparticle interference — •Zhixiang Sun[1], Pranab Kumar Nag[1], Danny Baumann[1], Rhea Kappenberger[1], Sabine Wurmehl[1,2], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

In spite of many theoretical and experimental efforts on studying the superconductivity of iron-based high temperature superconductors, the puzzle about LiFeAs's superconducting mechanism and pairing symmetry are still not clear. Here we want to present our low temperature scanning tunneling microscopy results on probing the superconductivity of LiFeAs. By taking conductance spectroscopic maps for both the superconducting state and normal state, we identify the scatterings due to the electron and hole bands close to the Fermi level. We observe a strong indication that the superconducting behavior in the hole bands are important for the formation of superconductivity in LiFeAs. Our results may also shine light on understanding the superconductivity in other iron pnictide superconductors.

TT 26: Focus Session: Engineered Magnetic Impurities: Interaction and Superconductivity

Future spintronic and quantum computing devices require magnetic nanostructures with specifically designed functionality. This focus session features theoretical aspects and experimental results on tunable properties of magnetic atoms and molecules on surfaces and artificial nanostructures in contact to normal metals and superconductors.

Organizers: Wolfgang Belzig (U Konstanz) and Katharina Franke (FU Berlin)

Time: Tuesday 9:30–12:15 Location: H20

Invited Talk TT 26.1 Tue 9:30 H20

Classical and quantum correlation induced bias asymmetries in coupled spin systems — •Markus Ternes — Max-Planck Institute for Solid State Research

In recent years inelastic spin-flip spectroscopy using a low-temperature scanning tunneling microscope has been a very successful tool for studying not only individual spins but also complex coupled systems. When these systems interact with the electrons of the supporting electrodes correlated many-particle states can emerge, making them ideal prototypical quantum systems. In this presentation I will show how the controlled coupling of individual spin systems can lead not only to an energy shift of the eigenstates reminiscent of an externally applied field, but also to a bias asymmetry in the differential conductance. Using $S = 1$ and $S = 1/2$ model systems of CoH_x on a h-BN/Rh(111) substrate [1] in conjunction with model Hamiltonians [2] which takes the coupling and correlation to the environment explicitly into account enables to precisely determine and control the emergence of correlations between the two subsystems on tip and sample.
[1] P. Jacobson et al. , Nature Communications **6**, 8536 (2015)
[2] M. Ternes, NJP **17**, 063016 (2015)

Invited Talk TT 26.2 Tue 10:00 H20

Magnetic anisotropy goes spintronic — •Maarten R. Wegewijs[1,2], Maciej Misiorny[3], and Michael Hell[4,5] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [2]Institute for Theory of Statistical Physics and JARA, RWTH Aachen, Germany — [3]Department of Microtechnology and Nanoscience MC2, Chalmers University of Technology, Göteborg, Sweden — [4]Division of Solid State Physics and NanoLund, Lund University, Sweden — [5]Center for Quantum Devices and Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, Denmark

Magnetic anisotropy of quantum spins as found in magnetic atoms and single-molecule magnets has traditionally been considered an intrinsic effect, generated locally by the combination of spin-orbit coupling and ligand field effects. In this talk I will show that magnetic anisotropy can appear in an entirely new way in very simple spintronic setups where a spin-isotropic quantum dot is exposed to the influence of magnetic electrodes. Magnetic anisotropy can thus appear as a dissipative transport quantity which is able to "pile up" in a system, quite similar to how spin accumulates in a spin-valve. Moreover, magnetic anisotropy can also be *generated from scratch* by coherent transport processes, resulting in a quadrupolar proximity effect [1], similar to the well-known controllable dipolar exchange field [2]. This turns an isotropic quantum spin $> 1/2$ into a full-blown single-molecule magnet with electrically controllable magnetic bistability.
[1] M. Misiorny, M. Hell , M. R. Wegewijs, Nature Phys. **9**, 801, (2013)
[2] M. Hell et al., PRB **91**, 195404 (2015)

Invited Talk TT 26.3 Tue 10:30 H20

Engineering the Kondo Effect in clean Carbon Nanotubes — •Christoph Strunk — Inst. f. Experimental and Applied Physics, University of Regensburg

Ultraclean carbon nanotubes (CNTs) form quantum dots of well-defined atomic structure at low temperatures. Transport spectroscopy of ground and excited states as a function of electron numbers in a parallel magnetic field results in detailed information about the band structures, in particular on spin-orbit and KK'-mixing effects.

This information is exploited in the analysis of the SU(4) Kondo effect [1] occurring at larger electron numbers, where the devices become more transmissive. The slightly broken fourfold degeneracy in our device gives rise to satellites of the Kondo peak that shift in a characteristic way in perpendicular and parallel magnetic field. Our observations reflect discrete symmetries of the CNT Hamiltonian, and are well reproduced by state of the art theoretical modeling [2].

On the other hand, multichannel electron interference is observed on the hole side of the CNT spectrum, where Coulomb effects are suppressed. A secondary interference effect is observed that provides information about the chiral angle of the CNTs by virtue of the trigonal warping of the underlying graphene band structure.

[1] P. Jarillo-Herrero et al., Nature **434**, 484 (2005)
[2] S. Smirnov and M. Grifoni, Phys. Rev. B **87**, 121302 (2013)

15 min. break

Invited Talk TT 26.4 Tue 11:15 H20

Majorana Fermions in Atomic Chains — •Ali Yazdani — Princeton University

In this talk, I will review the experimental progress in the realization of Majorana fermions in chains of magnetic atoms on the surface of a superconductor. Experimental results on the system of Fe on Pb(110) will be reviewed to show that this system has all the theoretically required criteria for hosting these exotic quasiparticles. We further show spectroscopic evidence for the presence of Majorana end modes in this system. The high resolution experimental signatures of their spatial structure agrees well with our detailed theoretical modeling of such edge modes. Finally, there has been proposal for detecting the spin signatures of these edge modes with spin polarized STM techniques. I will also describe our progress toward high resolution spin resolves measurements of the Majorana edge modes.

Invited Talk TT 26.5 Tue 11:45 H20

Magnetic adatoms on superconductors - a new venue for Majorana bound states? — •Felix von Oppen — Dahlem Center for Complex Quantum Systems & Fachbereich Physik, Freie Universität Berlin

In a recent experiment, Nadj-Perge et al.[1] (see also [2]) provide possible evidence for Majorana bound states in chains of magnetic adatoms on conventional superconductors. The formation of topological superconductivity in this system relies on ferromagnetic order of the magnetic moments and spin-orbit coupling provided by the substrate superconductor. In this talk, I will discuss the physical picture underlying this experiment, including an explanation of the unexpectedly strong localization of the observed end states [3,4], and will suggest additional experiments to probe the Majorana end states [5].

[1] S. Nadj-Perge et al., Science **346**, 602 (2014)
[2] M. Ruby, F. Pientka, Y. Peng, F. von Oppen, B. W. Heinrich, K. J. Franke, arXiv:1507.03104 (2015); to appear in PRL
[3] F. Pientka, L. I. Glazman, F. von Oppen, PRB **88**, 155420 (2013)
[4] Y. Peng, F. Pientka, L. I. Glazman, F. von Oppen, PRL **114**, 106801 (2015)
[5] Y. Peng, F. Pientka, Y. Vinkler-Aviv, L. I. Glazman, F. von Oppen, arXiv:1506.06763 (2015)

TT 27: Transport: Quantum Coherence and Quantum Information Systems - Theory 1 (Joint session of HL, MA and TT organized by TT)

Time: Tuesday 9:30–12:45 Location: H22

TT 27.1 Tue 9:30 H22

Measurement-induced entanglement of two transmon qubits by a single photon — Christoph Ohm and •Fabian Hassler — JARA Institute for Quantum Information, RWTH Aachen University, 52056 Aachen

On-demand creation of entanglement between distant qubits is desirable for quantum communication devices but so far not available for superconducting qubits. We propose an entanglement scheme that allows for single-shot deterministic entanglement creation by detecting a single photon passing through a Mach-Zehnder interferometer with one transmon qubit in each arm. The entanglement production essentially relies on the fact that superconducting microwave structures allow to achieve strong coupling between the qubit and the photon. By detecting the photon via a photon counter, a parity measurement is implemented and the wave function of the two qubits is projected onto a maximally entangled state. Moreover, due to the indivisible nature of single photons, our scheme promises full security for entanglement-based quantum key distribution.

TT 27.2 Tue 9:45 H22

Quantum Chemistry on a Superconducting Quantum Processor — •Michael P. Kaicher[1], Frank K. Wilhelm[1], and Peter J. Love[2] — [1]Theoretical Physics, Saarland University, 66123 Saarbruecken, Germany — [2]Department of Physics and Astronomy, Tufts University, Medford, MA 02155, USA

Quantum chemistry is the most promising civilian application for quantum processors to date. We study its adaptation to superconducting (sc) quantum systems, computing the ground state energy of LiH through a variational hybrid quantum classical algorithm. We demonstrate how interactions native to sc qubits further reduce the amount of quantum resources needed, pushing sc architectures as a near-term candidate for simulations of more complex atoms/molecules.

TT 27.3 Tue 10:00 H22

Optimization of Quantum Microwave Photodetection for circuit QED applications — •Marius Schöndorf[1], Luke C. Govia[1,3], Maxim Vavilov[2], Robert McDermott[2], and Frank K. Wilhelm[1] — [1]Universität des Saarlandes, Saarbrücken, Deutschland — [2]University of Wisconsin, Madison, USA — [3]McGill University, Montreal, Canada

Superconducting qubits are a promising candidate architecture for quantum computing and information. Readout of the qubit state is an important step that has to be taken for realising quantum algorithms in experiment. Recently we presented a qubit readout scheme [1] using a device called Jospehson Photomultiplier (JPM) [2]. One main step in this architecture is to read out a light state of a transmission line with the JPM. In this work we present a guide how to tune the different parameters in the experiment to optimize the measurement efficiency. We use Input-Output Theory to look at a continuous driven transmission line as well as various pulse states. Using analytical and numerical mehtods, we calculate conditions on the different parameters to optimize the respective measurement.

[1] L. C. G. Govia et al., PRA **92**, 022335 (2015)
[2] Y.-F. Chen et al., PRL **107**, 217401 (2012)

TT 27.4 Tue 10:15 H22

Theory and practice of dressed coherent states in circuit QED — •Frank Wilhelm[1] and Luke C. G. Govia[1,2] — [1]Theoretical Physics, Saarland University, Campus E 2.6, 66123 Saarbrücken, Germany — [2]Department of Physics, McGill University, Montreal, Canada

In the dispersive regime of qubit-cavity coupling, classical cavity drive populates the cavity, but leaves the qubit state unaffected. However, the dispersive Hamiltonian is derived after both a frame transformation and an approximation. Therefore, to connect to external experimental devices, the inverse frame transformation from the dispersive frame back to the lab frame is necessary. We show that in the lab frame the system is best described by an entangled state known as the dressed coherent state, and thus even in the dispersive regime, entanglement is generated between the qubit and the cavity. Also, we show that further qubit evolution depends on both the amplitude and phase of the dressed coherent state. This provides a limitation to readout in the dispersive regime. We show that only in the limit of infinite measurement time is this protocol QND, as the formation of a dressed coherent state in the qubit-cavity system applies an effective rotation to the qubit state. We show how this rotation can be corrected by

a unitary operation, leading to improved qubit initialization by measurement and unitary feedback.

[1] L. C. G. Govia and F.K. Wllhelm,
Phys. Rev. Appl. **4**, 054001 (2015)
[2] L. C.G. Govia and F.K. Wilhelm, arXiv: 1506.04997

TT 27.5 Tue 10:30 H22

Gradient optimization for analytic controls — •Elie Assémat[1], Shai Machnes[2], David Tannor[2], and Frank Wilhelm-Mauch[1] — [1]Saarland University, Saarbrücken, Germany — [2]Weizmann Institute of Science, Rehovot, Israël

Quantum optimal control becomes a necessary step in a growing number of studies in the quantum realm. Recent experimental advances showed that superconducting qubits can be controlled with an impressive accuracy. However, most of the standard optimal control algorithms are not designed to manage such high accuracy. To tackle this issue, a novel quantum optimal control algorithm have been introduced: the Gradient Optimization for Analytic conTrols (GOAT). It avoids the piecewise constant approximation of the control pulse used by standard algorithms. This allows an efficient implementation of very high accuracy optimization. It also includes a novel method to compute the gradient that provides many advantages, e.g. the absence of backpropagation or the natural route to optimize the robustness of the control pulses. This talk will present the GOAT algorithm and a few applications to transmons systems.

TT 27.6 Tue 10:45 H22

Optimal control of single flux quantum (SFQ) pulse sequences — •Per J. Liebermann and Frank K. Wilhelm — Universität des Saarlandes, Saarbrücken

Single flux quantum (SFQ) pulses are a natural candidate for on-chip control of superconducting qubits [1]. High accuracy quantum gates are accessible with quantum optimal control methods. We apply trains of SFQ pulses to operate single qubit gates, under the constraint of fixed amplitude and duration of each pulse. Timing of the control pulses is optimized using genetic algorithms and simulated annealing, decreasing the average fidelity error by several orders of magnitude. Furthermore we are able to reduce the gate time to the quantum speed limit. Leakage out of the qubit subspace as well as timing errors of the pulses are considered, exploring the robustness of our optimized sequence. This takes us one step further to a scalable quantum processor.

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

TT 27.7 Tue 11:00 H22

Nonlinearities in Josephson-Photonics — •Björn Kubala and Joachim Ankerhold — Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany

Embedding a voltage-biased Josephson junction within a high-Q superconducting microwave cavity provides a new way to explore the interplay of the tunneling transfer of charges and the emission and absorption of light. While for weak driving the system can be reduced to simple cases, such as a (damped) harmonic or parametric oscillator, the inherent nonlinearity of the Josephson junction allows to access regimes of strongly non-linear quantum dynamics.

Classically, dynamical phenomena such as thresholds for higher-order resonances, other bifurcations, and up- and down-conversion have been found [1]. Here, we will investigate how and to which extent these features appear in the deep quantum regime, where charge quantization effects are crucial. Theory allows to employ phase-space quantities, such as the Wigner-density of the cavity mode(s) [2], but also observables amenable to more immediate experimental access, such as correlations in light emission and charge transport, to probe these novel non-equilibrium transitions.

[1] S. Meister, M. Mecklenburg, V. Gramich, J. T. Stockburger, J. Ankerhold, B. Kubala, PRB **92**, 174532 (2015).
[2] A. D. Armour, B. Kubala, J. Ankerhold, PRB **91**, 184508 (2015).

15 min. break

TT 27.8 Tue 11:30 H22

Normal-metal quasiparticle traps for superconducting qubits — •Amin Hosseinkhani — Peter Grunberg Institute (PGI-2), Forschungszentrum Julich, D-52425 Julich, Germany — JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany

Superconducting qubits are promising candidates to implement quantum computation, and have been a subject of intensive research in the past decade. Excitations of a superconductor, known as quasiparticles, can reduce the qubit performance by causing relaxation; the relaxation rate is proportional to the density of quasiparticles tunneling through Josephson junction. Here, we consider engineering quasiparticle traps by covering parts of a superconducting device with normal-metal islands. We utilize a phenomenological quasiparticle diffusion model to study both the decay rate of excess quasiparticles and the steady-state profile of the quasiparticle density in the device. We apply the model to various realistic configurations to explore the role of geometry and location of the traps.

TT 27.9 Tue 11:45 H22

Decoherence and Decay of Two-level Systems due to Non-equilibrium Quasiparticles — •Sebastian Zanker, Michael Marthaler, and Gerd Schön — Karlsruher Institut für Technologie, Institut für Theoretische Festkörperpgysik, Karlsruhe, Deutschland

It is frequently observed that even at very low temperatures the number of quasiparticles in superconducting materials is higher than predicted by standard BCS-theory. These quasiparticles can interact with two-level systems, such as superconducting qubits or two-level systems (TLS) in the amorphous oxide layer of a Josephson junction. This interaction leads to decay and decoherence of the TLS, with specific results, such as the time dependence, depending on the distribution of quasiparticles and the form of the interaction. We study the resulting decay laws for different experimentally relevant protocols.

TT 27.10 Tue 12:00 H22

Theory of the double Quantum-dot Maser — •Clemens Müller and Thomas M. Stace — ARC Centre of Excellence for Engineered Quantum Systems, The University of Queensland, Brisbane, Australia

We consider a voltage-biased double quantum-dot (DQD) in the transport regime, dipole-coupled to a superconducting microwave cavity [1, 2]. We explore the effect of dissipative coupling of the DQD to a phononic environment and its influence on microwave gain and loss observed in the resonator. To this end, we develop a rate equation based on fourth-order perturbation theory in the dissipative and coherent DQD interactions. We compare our findings with the recent paper Ref.[3], where a different technique based on the Polaron transformation was used.

[1] Y.-Y. Liu, K. D. Petersson, J. Stehlik, J. M. Taylor, and J. R. Petta, PRL **113**, 036801 (2014)
[2] Y.-Y. Liu, J. Stehlik, C. Eichler, M. J. Gullans, J. M. Taylor, J. R. Petta, Science **347**, 285 (2015)
[3] M. J. Gullans, Y.-Y. Liu, J. Stehlik, J. R. Petta, J. M. Taylor, PRL **114**, 196802 (2015)

TT 27.11 Tue 12:15 H22

Upper bound for SL-invariant entanglement measures for mixed states of arbitrary rank — •Andreas Osterloh — Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany.

I present an algorithm that calculates an SL-invariant entanglement measure E as the threetangle of a mixed state of arbitrary rank. It is an alternative algorithm to ref. [1] and exploits the knowledge obtained for the rank-two case [2,3]. Whereas the known algorithm has an advantage of taking into consideration the whole range of the density matrix ρ, it on the other hand has the disadvantage of searching in a high-dimensional Hilbert space. Here, I only consider ensembles of two states each time but then calculate the upper bound obtained by the method presented in [2,3]. I discuss examples where the advantage of the new algorithm is obvious, but also highlight the obvious disadvantage of only considering rank two parts of ρ.

[1] S. Rodriques, N. Datta, and P. Love, PRA **90**, 012340 (2014)
[2] R. Lohmayer, A. Osterloh, J. Siewert, and A. Uhlmann, PRL **97**, 260502 (2006)
[3] A. Osterloh, J. Siewert, and A. Uhlmann, PRA **77**, 032310 (2008).

TT 27.12 Tue 12:30 H22

Occupation number entanglement in mesoscopic conductors — •David Dasenbrook[1] and Christian Flindt[2] — [1]Université de Genève, Genève, Switzerland — [2]Aalto University, Finland

The controlled entanglement of electrons in mesoscopic conductors has been theoretically investigated before using the spin- and orbital degrees of freedom. By contrast, entanglement of two spatially sepa-

rated electronic channels using the fermionic occupation number has mostly been considered inaccessible due to the charge superselection rule. However, using non-local measurements or combining several copies of occupation number entangled states, the superselection rules can be lifted and the entanglement can be detected using current and noise measurements. We present the theory for an interferometric setup to detect entanglement in the electron-hole degree of freedom of electronic excitations[1] as well as a mesoscopic setup that demonstrates entanglement and nonlocality of a single electron[2].

[1] D. Dasenbrook and C. Flindt, PRB **92**, 161412(R) (2015)
[2] D. Dasenbrook, J. Bowles, J. Bohr Brask, P. P. Hofer, C. Flindt, and N. Brunner, arXiv:1511.04450 (2015)

TT 28: Correlated Electrons: Quantum-Critical Phenomena - Experiment

Time: Tuesday 10:00–13:00 Location: H21

TT 28.1 Tue 10:00 H21

Quantum multicriticality in $Sr_3Ru_2O_7$ — •Dan Sun[1], Andreas Rost[2], Robin Perry[3], Manuel Brando[1], and Andrew Mackenzie[1,4] — [1]Max-Planck Institute for Chemical Physics of Solids, Noethnitzerstr. 40, Dresden, 01187, Germany — [2]Max-Planck Institute for Solid State Research, Heisenbergstraße 1, Stuttgart, 70569, Germany — [3]University College London, Gower Street, London, WC1E 6BT, United Kingdom — [4]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St. Andrews, North Haugh, St. Andrews KY16 9SS, United Kingdom

The low temperature phase diagram of the layered perovskite metal $Sr_3Ru_2O_7$ is of considerable interest because of the interplay between phase formation and quantum criticality [1,2]. We have performed high resolution specific heat and magnetocaloric measurements down to temperatures as low as 65 mK, uncovering evidence that a feature at 7.5 T previously thought to be a crossover is a quantum critical point resulting from the suppression towards T=0 of an extremely low energy scale. Additionally, we report for the first time the observation of thermodynamic signatures associated with the appearance of incommensurate magnetic order recently reported in neutron scattering measurements [3].

[1] S. Grigera et al. Science **306**, 1154 (2004)
[2] R. Borzi et al. Science **315**, 214 (2007)
[3] C. Lester et al. Nature Materials **14**, 373 (2015)

TT 28.2 Tue 10:15 H21

Effect of Uniaxial Strain on the Quantum Critical Phase of $Sr_3Ru_2O_7$ — •Mark E. Barber[1,2], Daniel O. Brodsky[1,2], Clifford W. Hicks[2], Robin Perry[3], 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]School of Physics and Astronomy, University of Edinburgh, Edinburgh EH9 3FD, United Kingdom

$Sr_3Ru_2O_7$ has a metamagnetic quantum critical endpoint, which in highly pure samples is masked by a novel phase. This phase is isotropic in the absence of symmetry-breaking fields, but weak in-plane magnetic fields are well-known to induce strong resistive anisotropy, leading to speculation that the phase intrinsically breaks the tetragonal symmetry of the lattice. We have used uniaxial strain to break the symmetry of the lattice and have found a dramatic response: compression by 0.1%, for example, induces a resistive anisotropy of ~ 2.5. I will discuss these results in the context of the underlying symmetry of the anomalous phase.

TT 28.3 Tue 10:30 H21

Optical Conductivity of Layered Ruthenates: The Role of Spin-Orbit Coupling and Coulomb Anistropy — •Esmaeel Sarvestani, Guoren Zhang, Evgeny Gorelov, and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Juelich, D-52425 Juelich, Germany

We use the combination of density functional theory and dynamical mean-field theory (LDA+DMFT) to calculate the optical conductivity of the layered ruthenates Sr_2RuO_4 and $Sr_3Ru_2O_7$. The calculations are performed via linear response theory and Kubo's formalism. For Sr_2RuO_4 two sets of interaction parameters, (U,J)=(2.3,0.4)eV and (3.1,0.7)eV, both commonly employed for ruthenates, are used. We show that including the spin-orbit coupling improves the agreement with experimental data. Finally, we analyze the effects of low-symmetry Coulomb interaction.

TT 28.4 Tue 10:45 H21

Quantum oscillation measurements of β-$LuAlB_4$ — Pascal Reiss[1], •Jordan Baglo[1], Xiaoye Chen[1], HongEn Tan[1], Michael Sutherland[1], Sven Friedemann[2], Swee K. Goh[3], Kentaro Kuga[4], Hisatomo Harima[5], Satoru Nakatsuji[4], and F. Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom — [2]HH Wills Laboratory, University of Bristol, Bristol, United Kingdom — [3]Chinese University of Hong Kong, Shatin, N.T., Hong Kong — [4]Institute for Solid State Physics, University of Tokyo, Kashiwa, Japan — [5]Department of Physics, Graduate School of Science, Kobe University, Kobe, Japan

The Yb-based heavy fermion superconductor β-$YbAlB_4$ displays a quantum critical point without tuning by applied pressure, magnetic field, or doping, which has been attributed to an unusual renormalised band structure [1]. Quantum oscillation measurements of the Fermi surface in β-$YbAlB_4$ have so far proved inconclusive, motivating us to undertake a detailed study of the isostructural reference compound β-$LuAlB_4$, which in contrast to the Yb compound is characterised by a filled $4f$ shell. We present comprehensive results from rotation and mass studies in β-$LuAlB_4$, which broadly agree with band structure calculations and display moderate mass enhancements contrasting with the much larger enhancements seen in β-$YbAlB_4$ – further emphasising the important contribution of f electrons to the itinerant electron physics of β-$YbAlB_4$.

[1] A. Ramires *et al.*, PRL **109**, 176404 (2012).

TT 28.5 Tue 11:00 H21

High Pressure Quantum Oscillation Studies in the Metallised Mott Insulator NiS_2 — •Hui Chang[1], Jordan Baglo[1], Alix McCollam[2], Inge Leermakers[2], Sven Friedemann[3], Xiaoye Chen[1], Pascal Reiss[1], HongEn Tan[1], Monika Gamza[4], William Coniglio[5], Stanley Tozer[5], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK. — [2]High Field Magnet Laboratory, Nijmegen, The Netherlands. — [3]HH Wills Laboratory, University of Bristol, UK. — [4]Jeremiah Horrocks Institute, University of Central Lancashire, UK. — [5]NHMFL, Tallahassee, Florida, USA.

The transition from a metallic to a Mott insulating state is a long-standing theme of fundamental interest in condensed matter research. One of the most basic questions concerns the evolution of the Fermi surface and carrier mass in the correlated metallic state near the Mott transition. Quantum oscillation measurements present a direct probe of the Fermi surface, and pressure rather than doping should be used as the tuning parameter in this case. We investigate this question in the Mott insulator NiS_2, which becomes metallic at a modest pressure of 30kbar. Using the tunnel diode oscillator technique in conjunction with high pressure anvil cells, we have observed quantum oscillations at pressures between 38kbar and 46kbar in magnetic fields up to 31T. This enables us to resolve key elements of the Fermi surface of high pressure NiS_2 and to obtain estimates of the effective carrier mass, which is strongly enhanced over band structure values. Moreover, we discuss the evolution of the Fermi surface, carrier effective mass and relaxation time on approaching the Mott transition.

TT 28.6 Tue 11:15 H21

Fermi surface of NiS_2 — •Pascal Reiss[1], Hui Chang[1], Jordan Baglo[1], Sven Friedemann[2], and F Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, United Kingdom — [2]HH Wills Physics Laboratory, University of Bristol, United Kingdom

Upon application of hydrostatic pressure of roughly 30 kbar, NiS_2 is found to display a transition from a Mott insulating state with a weak ferromagnetic ordering into a metallic state with an antiferromagnetic ordering. In this talk, we will present the results of band structure calculations based on DFT which aim to describe the high-pressure state. In particular, we will study the size and the topology of the

Fermi surface in dependence of both the magnetic ordering and the intra-site Coulomb repulsion U. The predicted extremal orbits and band masses are compared with recently performed quantum oscillation measurements. This enables us to better understand the nature of the Mott insulator transition in NiS_2.

15 min. break

TT 28.7 Tue 11:45 H21

ACRT technique for the single crystal growth of the heavy fermion compound $YbRh_2Si_2$ — •Sebastian Witt, Kristin Kliemt, Constantin Butzke, and Cornelius Krellner — Goethe University Frankfurt, 60438 Frankfurt am Main, Germany

In the heavy fermion compound $YbRh_2Si_2$ the antiferromagnetic ordering below 70 mK close to a quantum criticial point is well-studied. Beneath the magnetic ordering a new phase transition was found recently at 2 mK. [1] It is necessary to prepare large and high-quality single crystals for studying the nature of this new phase transition. Besides the optimization of the single crystal growth it is important to investigate single crystals with different isotopes at this phase transition.

Here, we report the crystal growth of $YbRh_2Si_2$ with the accelerated crucible rotation technique (ACRT). ACRT shows for other compounds, e.g. YAG (yttrium aluminum garnet, $Y_3Al_5O_{12}$), that this technique can reduce flux impurities and enhance the yield of larger crystals. We also report the attempt to receive metallic isotopes of ytterbium with metallothermic reduction. Crystals with different isotopes of silicon and ytterbium can be used for NMR measurements to investigate the underlying phenomena of quantum criticality in more detail.

[1] Schuberth et al., J. Phys.: Conf. Ser. 150 (2009) 042178.

TT 28.8 Tue 12:00 H21

$YbNi_4P_2$: Single crystal growth by the Czochralski method and high-field magnetization measurements — •Kristin Kliemt[1], Tobias Förster[2], Manuel Brando[3], and Cornelius Krellner[1] — [1]Goethe-University, Frankfurt, Germany — [2]HLD, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]MPI for Chemical Physics of Solids, Dresden, Germany

We have investigated a new generation of $YbNi_4P_2$ single crystals that were grown from a levitating melt by the Czochralski method. With T_C= 0.17 K, this ferromagnetic material has the lowest Curie temperature ever observed among stoichiometric compounds [1]. A quantum critical point occurs in the substitution series $YbNi_4(P_{1-x}As_x)_2$ at $x \approx 0.1$ [2]. The hybridization between localized f-electrons and the conduction electrons leads to a Fermi-liquid ground state with narrow bands and strongly enhanced effective electronic masses (heavy fermion system, Kondo temperature 8 K). An external magnetic field can split the bands, deform the Fermi surface and simultaneously suppress the Kondo interaction. If such a deformation changes the topology, it is called a Lifshitz transition. Previous thermodynamic and electrical transport studies have found indications for Lifshitz transitions in this Kondo lattice system [3]. We report on results of high-field magnetization measurements at low temperature to further investigate the putative Lifshitz transitions in $YbNi_4P_2$.

[1] C. Krellner et al., NJP **13**, 103014 (2011)
[2] A. Steppke et al., Science **339**, 933 (2013)
[3] S. Friedemann, H. Pfau (unpublished)

TT 28.9 Tue 12:15 H21

Competing ground states in $LuFe_4Ge_2$ tuned by external pressure — •Mukkattu Omanakuttan Ajeesh, Katharina Weber, Ricardo dos Reis, Cristoph Geibel, and Michael Nicklas — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, Dresden, Germany

Tuning competing ground-state properties using external pressure has attracted much attention in current condensed matter research. This is due to the fact that exotic phenomena and unconventional phases occur in regions of competing energy scales. Here, we present an investigation on $LuFe_4Ge_2$ by electrical resistivity experiments under external pressure in order to understand the interplay between competing ground states in a frustrated, itinerant magnetic system. At ambient pressure $LuFe_4Ge_2$ orders antiferromagnetically below 32 K. The antiferromagnetic (AFM) transition is connected with a structural transition. We have established the temperature – pressure phase diagram: pressure suppresses the original antiferromagnetically ordered state to zero temperature at around 1.7 GPa. Upon further increasing pressure a new pressure-induced phase emerges. This phase exhibits a qualitatively different magnetoresistance compared with the AFM phase suggesting a different type of ordering than at lower pressures. Furthermore, above 1.5 GPa we find a metamagnetic transition at higher magnetic fields. The onset of this phase shifts to lower fields with increasing pressure. Further studies to understand the nature of the new phases are on the way.

TT 28.10 Tue 12:30 H21

CePdAl - a frustrated Kondo lattice at a quantum critical point — •Veronika Fritsch[1,2], Akito Sakai[1], Zita Hüsges[3], Stefan Lucas[3], Wolfram Kittler[2], Christian Taubenheim[2], Kai Grube[2], Chien-Lung Huang[2,3], Philipp Gegenwart[1], Oliver Stockert[3], and Hilbert v. Löhneysen[2] — [1]EP 6, Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Karlsruhe Institute of Technology, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

CePdAl is one of the rare frustrated Kondo lattice systems that can be tuned across a quantum critical point (QCP) by means of chemical pressure, i. e., the substitution of Pd by Ni [1]. Magnetic frustration and Kondo effect are antithetic phenomena: The Kondo effect with the incipient delocalization of the magnetic moments, is not beneficial for the formation of a frustrated state. On the other hand, magnetic frustrated exchange interactions between the local moments can result in a breakdown of Kondo screening [2]. Furthermore, the fate of frustration is unclear when approaching the QCP, since there is no simple observable to quantify the degree of frustration. We present thermodynamic and neutron scattering experiments on $CePd_{1-x}Ni_xAl$ close to the critical concentration $x \approx 0.14$. Our experiments indicate that even at the QCP magnetic frustration is still present, opening the perspective to find new universality classes at such a quantum phase transition.

[1] V. Fritsch *et al.*, PRB **89**, 054416 (2014).
[2] T. Senthil *et al.* PRB **69**, 035111 (2004).

TT 28.11 Tue 12:45 H21

Enhancement of effective Grüneisen parameter near structural quantum critical point in $(Ca_{0.9}Sr_{0.1})_3Rh_4Sn_{13}$ — •Rudra Sekhar Manna[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

The interplay between superconductivity and structural instabilities in quasi-skutterudite compounds is playing an important role in recent years. $Sr_3Rh_4Sn_{13}$ 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 $(Ca_xSr_{1-x})_3Rh_4Sn_{13}$. A structural quantum phase transition occurs at a critical concentration x_c = 0.9. The specific heat for x_c = 0.9, measured in a magnetic field to suppress superconductivity indicates a pronounced enhancement of the phonon (T^3) contribution at low-temperature compared to the x = 0 sample, possibly related to the softening of an optical phonon mode [1, 2]. We have performed high-resolution thermal expansion and specific heat measurements on a lump of small $(Ca_{0.9}Sr_{0.1})_3Rh_4Sn_{13}$ crystals. Thermal expansion shows a huge enhancement of phonon contribution compared to x = 0 sample. Moreover, the effective Grüneisen parameter $\Gamma_{eff} = \beta \cdot V_{mol}/\kappa_T \cdot C$ displays a significant enhancement upon cooling, indicative of quantum criticality.

[1] S. K. Goh *et al.*, PRL **114**, 097002 (2015).
[2] W. C. Yu *et al.*, PRL **115**, 207003 (2015).

TT 29: Topology- and Symmetry-Protected Materials (Joint session of DS, HL, MA, O and TT organized by O)

Time: Tuesday 10:30–13:30 Location: S051

Invited Talk TT 29.1 Tue 10:30 S051

Toward single atom qubits on a surface: Pump-probe spectroscopy and electrically-driven spin resonance — •William Paul — IBM Research, San Jose CA, USA

We will discuss the characterization of spin dynamics by pump-probe spectroscopy and the use of gigahertz-frequency electric fields to drive spin resonance of a Fe atom on a MgO/Ag(001) surface. Also, the technical challenges in applying a precise voltage to the tip sample junction across a wide radio-frequency bandwidth will be described. The energy relaxation time, T1, of single spins on surfaces can be measured by spin-polarized pump-probe STM (scanning tunneling microscopy) [1]. To date, the relaxation times reported for Fe-Cu dimers on Cu2N insulating films have been of the order ˜100 ns [1]. A three-order-of-magnitude enhancement of lifetime, to ˜200 us, was recently demonstrated for Co on a single-monolayer of MgO [2]. Here, we report on the tailoring of the T1 lifetime of single Fe atoms on single- and multi- layer MgO films grown on Ag(001). Next, we demonstrate electron spin resonance of an individual single Fe atom, driven by a gigahertz-frequency electric field applied across the tip-sample junction, and detected by a spin-polarized tunneling current. The principle parameters of the spin resonance experiment, namely the phase coherence time T2 and the Rabi rate, are characterized for Fe atoms adsorbed to the monolayer MgO film.

[1] Loth et al., Science 329, 1628 (2010) [2] Rau and Baumann et al., Science 344, 988 (2014) [3] Baumann and Paul et al., Science 350, 417 (2015)

TT 29.2 Tue 11:00 S051

Mesoscopic spin coherence through electron focusing in topological insulators — •Philipp Rüssmann, Phivos Mavropoulos, Nguyen H. Long, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Long coherence lengths of quasiparticles are an essential ingredient for spintronics applications. Motivated by previous experiments [P. Sessi et al, Nat. Comm. 5, 5349 (2014)] we undertook a combined theoretical and experimental study, using density functional theory and STM, where we found standing wave patterns of mesoscopic dimensions around magnetic defects on the surface of Bi_2Te_3. We identified two necessary conditions for the effect: (i) focusing by the Bi_2Te_3 Fermi surface due to its hexagonal warping and (ii) large scattering strength of the magnetic defects. We modeled different magnetic defects and analyzed the energy dependence of the scattering properties in the energy range where the shape of the constant energy contour changes from circular over hexagonal to snowflake-like. For the calculation of the electronic structure and scattering properties we employed the full-potential relativistic Korringa-Kohn-Rostoker Green-function method [D.S.G. Bauer, Schriften des Forschungszentrums Jülich, Key Tech. 79 (2014); N. H. Long et al., Phys. Rev. B 90, 064406 (2014)].

We enjoy close collaborations with P. Sessi and M. Bode (Würzburg University) and thank for financial support from the DFG (SPP-1666), the VITI project of the Helmholtz Association and computational support from the JARA-HPC Centre (RWTH Aachen University).

TT 29.3 Tue 11:15 S051

Generation of transient photocurrents in the topological surface state of Sb_2Te_3 bydirect optical excitation with mid-infrared pulses — •Johannes Reimann, Kenta Kuroda, Jens Güdde, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg

We combine tunable mid-infrared (MIR) pump pulses with time- and angle-resolved two-photon photoemission (2PPE) to study the ultrafast electron dynamics of the topological surface state (TSS) of Sb_2Te_3. It is revealed that MIR pulses permit a direct excitation of the unoccupied TSS owing to an optical coupling across the Dirac point. This is in contrast to the delayed filling observed in previous 2PPE experiments on topological insulators with pump photon energies in the visible range. The novel optical coupling provokes asymmetric transient populations of the TSS at $\pm k_{||}$, which mirrors a macroscopic photoexcited electric surface current. By observing the decay of the asymmetric population, we directly investigate the dynamics of the photocurrent in the time domain. We find a long equilibration time of $\tau_k^e = 2.5$ ps for the population at $\pm k_{||}$ that shows no significant change for different sample temperatures of 80 K and 300 K. Considering a Debye temperature of $\theta_D = 162$ K this result indicates that phonons play only a minor role for the momentum scattering. We suggest that scattering at surface defects is instead the limiting factor for the current lifetime.

TT 29.4 Tue 11:30 S051

Time- and angle-resolved two-photon photoemission from p-doped septuple-layered topological insulators — •Sebastian Otto, Jonas Rietsch, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Time- and angle-resolved two-photon photoemission is used to study the electronic structure of septuple-layered antimony telluride crystals of different p-dopings. All surfaces show a topological surface state. The Dirac point is found between $E_F + 0.38$ eV for $GeSb_2Te_4$ and $E_F + 0.25$ eV for $SnBi_{0.2}Sb_{1.8}Te_4$. The topological surface state is populated mainly from the conduction band minimum according to the evolution of its temporal population. Similar to the case of $SnSb_2Te_4$ [1], the electrons in the topological surface state decay rather fast into a partially unoccupied valence band maximum depending on the strength of the p-doping.

[1] D. Niesner, S. Otto, V. Hermann and Th. Fauster, Phys. Rev. B **89**, 081404(R) (2014)

TT 29.5 Tue 11:45 S051

Controlling the spin-texture of topological insulators with organic molecules — Sebastian Jakobs[1,2], Benjamin Stadtmüller[1], •Dominik Jungkenn[1], Martin Laux[1], Johannes Stöckl[1], Martin Aeschlimann[1], Stefan Mathias[3], and Mirko Cinchetti[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Str 46, 67663 Kaiserslautern, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Erwin Schroedinger Straße 46, 67663 Kaiserslautern, Germany — [3]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

We present a rational design approach to customize the spin texture of surface states of a topological insulator (TI). This approach relies on the extreme multifunctionality of organic molecules that are used to functionalize the surface of the prototypical TI Bi2Se3. For the rational design we use theoretical calculations to guide the choice and chemical synthesis of appropriate molecules that customize the spin texture of Bi2Se3. The theoretical predictions are then verified in angular-resolved photoemission experiments. We show that the surface can be passivated while the Dirac cone can be shifted at will by tuning the strength of the molecule-TI interaction and Rashba-split quantum-well interface states can be created. These tailored interface properties - passivation, spin-texture tuning and creation of hybrid interface states - open a wide field of opportunities for interface assisted molecular spintronics in spin-textured materials.

TT 29.6 Tue 12:00 S051

Modulating the spin polarization of photoelectrons from a topological insulator — •Ji Hoon Ryoo and Cheol-Hwan Park — Department of Physics, Seoul National University 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Korea

It has been predicted that the spin polarization of photoelectrons emitted from a topological insulator is highly tunable so that almost 100 % polarization along any arbitrary direction can be achieved by tuning the polarization of light [1]. There have been a number of experimental confirmations of this photo-induced spin modulation phenomenon [2-6]. Although this photo-induced spin modulation in topological insulators suggests a new kind of spin-polarized electron sources [2], there have been some experimental results that cannot be explained by previous theoretical descriptions [1]. In this presentation, we theoretically investigate photoemission process from topological insulators and interpret the recent experimental observations.

[1] C.-H. Park, S. G. Louie, Phys. Rev. Lett. 109, 097601 (2012).

[2] C. Jozwiak et al., Nat. Phys. 9, 293 (2013).
[3] Z.-H. Zhu et al., Phys. Rev. Lett. 112, 076802 (2014).
[4] Z. Xie et al., Nat. Commun. 5, 3382 (2014).
[5] Y. Cao et al., arXiv:1211.5998v1
[6] J. Sánchez-Barriga et al., Phys. Rev. X 4, 011046 (2014).

TT 29.7 Tue 12:15 S051

Dirac Cone Protected by Non-Symmorphic Symmetry and highly dispersive 3D Dirac crossings in ZrSiS — •Leslie Schoop[1], Mazhar Ali[2], Carola Strasser[1], Viola Duppel[1], Stuart Parkin[2], Bettina Lotsch[1], and Christian Ast[1] — [1]Max Planck Insititut für Festkörperforschung, Stuttgart — [2]Max Planck Institut für Mikrostrukturphysik, Halle

Materials harboring exotic quasiparticles, such as Dirac and Weyl fermions have garnered much attention from the physics and material science communities. Here, we show with angle resolved photoemission studies supported by ab initio calculations that the highly stable, non-toxic and earth-abundant material, ZrSiS, has an electronic band structure that hosts several Dirac cones which form a Fermi surface with a diamond-shaped line of Dirac nodes. We also experimentally show, for the first time, that the square Si lattice in ZrSiS is an excellent template for realizing the new types of 2D Dirac cones protected by non-symmophic symmetry and image an unforseen surface state that arises close to the 2D Dirac cone. Finally, we find that the energy range of the linearly dispersed bands is as high as 2 eV above and below the Fermi level; much larger than of any known Dirac material so far. We will discuss why these characteristics make ZrSiS very promising for future applications.

TT 29.8 Tue 12:30 S051

2D Dirac cones protected by non-symmorphic symmetry in ZrSiS and ZrSiTe — •Andreas Topp[1], Leslie M. Schoop[1], Carola Strasser[1], Bettina V. Lotsch[1,2,3], and Christian R. Ast[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Department of Chemistry, Ludwig-Maximilians-Universität, D-81377 München — [3]Nanosystems Initiative Munich (NIM) & Center for Nanoscience, D-81377 München

Three-dimensional Dirac semimetals which accommodate massless Dirac and Weyl fermions, have recently become of considerable interest because of their exotic physical properties, e.g. an extremly high mobility and magnetoresistance. A new compound, ZrSiS, hosting a square lattice of Si atoms, has been shown to host 3D Dirac cones at the Fermi level with a very large energy range of linear dispersion [1]. Additionally, a new type of Dirac cone protected by non-symmorphic symmetry has been found to exist below the Fermi level which was predicted theoretically to exist in a square lattice [2]. Here, we show by *ab initio* calculations, that in the compound ZrSiTe this cone is moved to the Fermi level. We present the crystal growth results and show preliminary ARPES data concerning the electronic structure of these two compounds.

[1] L. M. Schoop *et al.*, arXiv preprint arXiv:1509.00861 (2015).
[2] S. M. Young, and C. L. Kane, Phys. Rev. Lett. 115, 126803 (2015).

TT 29.9 Tue 12:45 S051

Resonant photoemission of the spin-polarized electronic structure in strongly spin-orbit coupled systems — •Henriette Maass, Hendrik Bentmann, Christoph Seibel, Thiago R. F. Peixoto, and Friedrich Reinert — Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg

Strong spin-orbit coupling leads to a lifting of the spin degeneracy in the electronic structure and the emergence of novel topological phases in non-centrosymmetric environments, such as interfaces or surfaces. Using resonant angle-resolved photoemission experiments (ARPES) we have investigated the spin-polarized electronic structure in the surface alloy $BiAg_2/Ag(111)$ and the topological insulator Bi_2Te_3.

Our data reveals pronounced momentum dependent modulations of the photoemission intensity in the 6p derived surface states of $BiAg_2/Ag(111)$, when the photon energy is tuned across the Bi 5d core level excitation. In particular a complete suppression of spectral weight of spin-up and spin-down valence bands occurs for energies shortly below the Bi $5d_{5/2}$ and the $5d_{3/2}$ core levels, respectively. At the same time a considerable modification of the photoelectron spin-polarization can be observed. We compare these results to the case of the topological insulator Bi_2Te_3, where similar variations in the photoemission intensity occur.

[1] H. Bentmann *et al.*, arXiv 1507.04664

TT 29.10 Tue 13:00 S051

Electronic structure and topology of the natural superlattice phase $Bi_1Te_1 = (Bi_2)_1(Bi_2Te_3)_2$ — •Markus Eschbach[1], Martin Lanius[1], Ewa Mlynczak[1], Jens Kellner[2], Chengwang Niu[1], Peter Schüffelgen[1], Mathias Gehlmann[1], Pika Gospodaric[1], Sven Döring[1], Martina Luysberg[1], Gregor Mussler[1], Gustav Bihlmayer[1], Markus Morgenstern[2], Detlev Grützmacher[1], Lukasz Plucinski[1], and Claus M. Schneider[1] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institut, 52425 Jülich, Germany — [2]II. Physikalisches Institut B, RWTH Aachen University, 52074 Aachen, Germany

We report on experimental and theoretical investigations of thin films of Bi_1Te_1 grown on Si(111), being part of the natural supperlattice phase series $[Bi_2]_x[Bi_2Te_3]_y$ with $x = 1$ and $y = 2$. Contrary to the closely related, prototypical 3D strong topological insulator Bi_2Te_3, its electronic strutcture as well as topological properties have not been adressed so far. In this study, we present detailed characterization of the bulk crystal structure by X-ray diffraction and transmission electron microscopy and the surface chemistry by X-ray photoelectron spectroscopy. The rich surface electronic structure, investigated by spin- and angle-resolved photoemission spectroscopy, reveals surface states that can be easily confused with Dirac cone-like topological surface states. However, we will show by experiment and comprehensive ab inito density functional theory calculations that Bi_1Te_1 is a weak topological insulator.

TT 29.11 Tue 13:15 S051

Probing the electronic structure of the magnetic topological insulator $(BiSbV)_2Te_3$ with soft X-ray photoelectron spectroscopy — •Thiago Ribeiro Fonseca Peixoto[1,3], Mohammed Al-Baidhani[1,3], Henriette Maass[1,3], Christoph Seibel[1,3], Hendrik Bentmann[1,3], Steffen Schreyeck[2,3], Martin Winnerlein[2,3], Stefan Grauer[2,3], Charles Gould[2,3], Karl Brunner[2,3], Laurens Molenkamp[2,3], and Friedrich Reinert[1,3] — [1]EP VII, Fakultät f. Physik u. Astronomie, Uni-Würzburg — [2]EP III, Fakultät f. Physik u. Astronomie, Uni-Würzburg — [3]Röntgen Center for Complex Materials (RCCM), Uni-Würzburg

By means of X-ray photoemission (XPS) and absorption (XAS) spectroscopy we investigated the electronic structure of $(BiSbV)_2Te_3$ thin films, a three-dimensional magnetic topological insulator, recently reported as an anomalous quantum Hall system [1]. The films were epitaxially grown on a Si(111) crystal and covered by a Se cap to avoid contamination during exposition to air. After thermally desorbing the Se cap, the core-level lines of the constituent elements and the V $L_{2,3}$ absorption edges were measured for different V concentrations (0, 2 and 4 at.%). Our data evidence the incorporation of Se atoms in the film. By means of resonant photoemission we identify the signature of the V 3d states at the Fermi level, which may contribute to the exotic transport properties of the system. We discuss the chemical environment of the V atoms and show that our techniques are well suited for the study of the electronic properties of this novel class of materials.

[1] C.-Z. Chang *et al.*, Nat. Mat. Lett. **14**, 473 (2015).

TT 30: Superconductivity: Fe-based Superconductors - Theory

Time: Tuesday 11:00–13:00 Location: H19

Invited Talk TT 30.1 Tue 11:00 H19

Selective correlations and heavy-fermionic behaviour in Iron-based superconductors — •Luca de' Medici — European Synchrotron Radiation Facility, 71 Av. des Martyrs, 38000 Grenoble, France — Ecole Supérieure de Physique et Chimie industrielles de la Ville de Paris, 10 rue Vauquelin, 75005 Paris - France

The matching between recent experimental evidences from various probes and realistic theoretical calculations highlights the coexistence,

in the normal phase of Fe-based superconductors, of strongly correlated and weakly correlated electrons. This peculiar situation can be backtracked to the influence of Hund's coupling exchange interaction between the conduction electrons in these materials, and can be controlled to some degree. In some of these compounds this differentiation can get quite extreme and gives rise to heavy-fermionic behaviour. We will speculate that these and similar d-electron materials could constitute a new ballpark for the exploration of heavy-fermionic physics, and of its applications. A new possible application of the strong thermomagnetic properties that can in principle be found in heavy-fermions is proposed: self-cooling of high-current cables.

[1] L. de' Medici, G. Giovannetti and M. Capone, PRL **112**, 177001 (2014)
[2] L. de' Medici in *Iron-based Superconductivity*, Springer Series in Materials Science **211**, 2015, pp 409-441
[3] L. de' Medici, ArXiv:1506.01674

TT 30.2 Tue 11:30 H19

Hundness versus Mottness in a Three-Band Hund Model with Relevance for Iron-Pnictides — •Katharina M. Stadler[1], Zhiping Yin[2], Jan von Delft[1], Gabriel Kotliar[2], and Andreas Weichselbaum[1] — [1]Ludwig Maximilians University, Munich, Germany — [2]Rutgers University, New Jersey, USA

The recently discovered iron pnictide superconductors (as well as chalcogenides, ruthenates, and other 4d transition metal oxides) show puzzling anomalous properties, like a coherence-incoherence crossover, also in the normal state. While there is consensus about strong correlation effects playing a key role in these materials, their precise origin (Coulomb repulsion or Hund's rule coupling between electrons of different orbitals) has been under debate as one of the major open questions in the field many years. In a recent detailed study of the Hund metal problem [1] the coherence-incoherence crossover was shown to be connected to spin-orbital separation and to be clearly driven by Hund's rule coupling.
In order to better understand the differences between Mott insulators and Hund metals we explore the phase diagram for a three-band model with Coulomb repulsion and Hund's rule coupling on a Bethe lattice at 1/3 filling using the numerical renormalization group to obtain a numerically exact dynamical mean-field theory solution.

[1] K. M. Stadler et al., PRL **115**, 136401 (2015)

TT 30.3 Tue 11:45 H19

Current induced magnetic flux response in frustrated three-band superconductors as a bulk probe of broken time reversal symmetry (BTRS) ground states — Yuriy Yerin[1], Alexander Omelyanchouk[1], •Stefan-Ludwig Drechsler[2], Jeroen van den Brink[2], and Dmitri Efremov[2] — [1]Verkin Inst. for Low Temperature Physics and Engineering. 61103 Kharkiv, Ukraine — [2]Inst. for Theor. Solid State Physics at the Leibniz Inst. for Solid State an Materials Research, IFW-Dresden, D-01171 Dresden, Germany

Within the Ginzburg-Landau formalism we provide a classification of all possible ground states (GS) of a three-band superconductor (3BSC) where either frustrated states with BTRS or a single non-BTRS GS with unconventional/conventional s-wave symmetry, respectively, exist. The necessary condition for a BTRS GS in general cannot be reduced to a "-"sign of the product of all interband couplings (IBC) valid in the case of 3 equivalent bands with repulsive equal IBC, only. It corresponds to a maximal IBC frustration. We show that with increasing diversity of the parameter space this frustration is reduced and the regions of possible BTRS GS start to shrink. We track possible evolutions of a BTRS GS of a 3BSC based doubly-connected system in an external magnetic field. Depending on its parameters, a magnetic flux can induce various current density leaps, connected with adiabatic or non-adiabatic transitions from BTRS to non-BTRS states and vice versa. The current induced magnetic flux response of samples with a doubly-connected geometry e.g. as a thin tube provides a suitable experimental tool for the detection of BTRS GS.

TT 30.4 Tue 12:00 H19

Dynamical coupled modes theory for an $s_{\pm}$-pairing mechanism of superconductivity in doped iron pnictides — Mikhail Kiselev[1], •Dmitry Efremov[2], Stefan-Ludwig Drechsler[2], Konstantin Kikoin[3], and Jeroen van den Brink[2] — [1]International Center for Theoretical Physics, I-34151 Trieste, Italy — [2]Institute for Theoretical Solid State Physics at the Leibniz Institute for Solid State an Materials Research Dresden, IFW-Dresden, D-01171 Dresden, Germany — [3]School of Physics and Astronomy, Tel Aviv University, 69978 Tel Aviv, Israel

We develop a high-temperature approach to the problem of the interplay between magnetic and superconducting phases in multi-band iron pnictides. A dynamical mode-mode coupling theory is derived from the the microscopic theory based on the solution of the coupled Bethe-Salpeter equations. We focus on the vicinity to a spin density wave (SDW) where spin fluctuations enhance the onset of superconducting ordering. Special attention is paid to arsenic deficient materials where As vacancies behaves as effective magnetic defects [1]. The proposed theory allows generalization to multi-mode regimes.

[1] K. Kikoin, S.-L. Drechsler, K. Koepernik, J. Málek, and J. van den Brink, Nature, Scientific Reports **5**, 11280 (2015).

TT 30.5 Tue 12:15 H19

Robust Determination of the Superconducting Gap Sign Structure via Quasiparticle Interference — •Dustin Altenfeld[1], Peter Hirschfeld[2], Ilya Eremin[1,3], and Igor Mazin[4] — [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]Kazan Federal University, Kazan 420008, Russian Federation — [4]Code 6393, Naval Research Laboratory, Washington, DC 20375, USA

Using an electronic theory, we present a qualitative description to identify sign changes of the superconducting order parameter via quasiparticle interference (QPI) measurement in Fe-based superconductors (FeSc). In particular, we point out that the temperature dependence of the momentum-integrated QPI data can be used to differentiate between s_{+-} and s_{++} states in a system with typical iron pnictide Fermi surface. We show that 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. We further suggest this method as a robust way of the determination of the superconducting gap sign structure in experiment and discuss its application to the LiFeAs compounds.

TT 30.6 Tue 12:30 H19

The role of the d-filling in DFT+DMFT calculations of pnictides containing Chromium — •Martin Edelmann[1], Luca de' Medici[2], Massimo Capone[3], Gianluca Giovannetti[3], and Giorgio Sangiovanni[1] — [1]ITPA Universitaet Wuerzburg, Wuerzburg, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France — [3]Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy

In the recent years, transition-metal-pnictides gained attention as among them there are new high-T_c superconductors. The physical effects are strongly influenced by the Hund's coupling and the extent of this influence directly depends on the orbital occupation. We calculate quasiparticle properties in Chromium-pnictide materials of different classes via DFT+DMFT. To this aim, we construct various localized bases, consisting of only the transition-metal d orbitals located around the chemical potential or also including ligands' p states. We then analyze the orbital-resolved quasiparticle weight and the scattering rates as well as modifications of the Fermi surfaces due to electronic correlation. These help in understanding why the electronic properties of the various families are compatible with a localized as well as an itinerant picture.

TT 30.7 Tue 12:45 H19

Spin-wave Excitations in Tetragonal and Orthorhombic Spin-Density-Wave Phases of Iron Pnictides — •Daniel David Scherer and Brian Møller Andersen — Niels Bohr Institute, University of Copenhagen, 2100, Copenhagen, Denmark

The most prominent and abundant spin-density-wave (SDW) state found theoretically and experimentally in the Fe-based superconductor materials features stripy orthorhombic magnetic order in the Fe layer with ordering vectors $\mathbf{Q}_1 = (\pi, 0)$ or $\mathbf{Q}_2 = (0, \pi)$. Recently, however, tetragonal magnetic orders have been discovered in these systems [1-4]. A candidate for a commensurate tetragonal SDW state is a spin- and charge-ordered state (SCO) that was previously understood [5,6] as a superposition of two stripy orders with an induced checkerboard charge order. Starting from a DFT-derived 5-orbital model for the electronic degrees of freedom, we here focus on a theoretical investigation of the spin-wave spectra in the orthorhombic stripy SDW and tetragonal SCO states within an itinerant weak-coupling approach, and present a comprehensive comparison of our results to experimental data.

[1] S. Avci et al., Nat. Commun. **5**, 3845 (2014).
[2] A. E. Böhmer et al., Nat. Commun. **6**, 7911 (2015).
[3] J. M. Allred et al., arXiv:1505.06175.
[4] L. Wang et al., arXiv:1510.03685.
[5] X. Wang and R. M. Fernandes, Phys. Rev. B **89**, 144502 (2014).
[6] M. N. Gastiasoro and B. M. Andersen, Phys. Rev. B **92**, 150506(R) (2015).

TT 31: Topological Insulators: Status Quo and Future Directions (Joint session of DS, MA, HL, O and TT organized by DS)

Time: Tuesday 12:30–13:00 Location: H8

TT 31.1 Tue 12:30 H8

Topological invariants in the embedding-potential — Hiroshi Ishida[2] and •Daniel Wortmann[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]College of Humanities and Sciences, Nihon University, Tokyo, Japan

The embedding potential[1] defined at the boundary of a semi-infinite crystal defines the boundary condition for the wavefunction and can be interpreted as its logarithmic derivative. We demonstrate how this embedding potential can be utilized to determine the Z_2 topological invariant in time-reversal invariant insulators and how the formation of the surface states can be understood in terms of properties of the embedding potential.

Besides the general ideas and the theory, numerical examples for simple topological insulators and trivial materials will be shown and compared.

[1] J.E.Inglesfield, J. Phys. C **14**, 3795 (1981)

TT 31.2 Tue 12:45 H8

Quantum-well stabilized two-dimensional topological crystalline insulators — Chengwang Niu, Patrick Buhl, •Gustav Bihlmayer, Daniel Wortmann, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

By means of density functional theory calculations, we find that monolayers of SnTe and PbTe can be characterized as two-dimensional topological crystalline insulators (2D-TCIs) with band gaps of 50 meV and 90 meV, respectively [1]. Embedded in NaCl or NaBr films, these 2D-TCIs are not only structurally stabilized, but also the band gaps can be enhanced up to 470 meV. Moreover, in these quantum-well structures the Madelung potential of the strongly ionic rocksalt lattice acting on the SnTe or PbTe layers enhances the band-inversion. Even in thicker, topologically trivial telluride films band-inversions can be induced that trigger a transition to a TCI state [2]. We further analyse the effect of an external magnetic (exchange) field on the SnTe and PbTe monolayers and find that the quantum anomalous Hall regime can be reached with fields exceeding 0.2 eV. This happens even for an in-plane oriented field where the mirror symmetry, protecting the TCI phase, is broken. We investigate the properties of the edge states for ribbons of different orientations using maximally localized Wannier functions.

Financial support of the DFG (SPP 1666) is gratefully acknowledged.

[1] C. Niu et al., Phys. Rev. B. **91**, 201401(R) (2015).
[2] C. Niu et al., submitted (2015).

TT 32: Transport: Topological Insulators - 3D (Joint session of DS, HL, MA, O and TT organized by TT)

Time: Tuesday 14:00–15:45 Location: H18

Invited Talk TT 32.1 Tue 14:00 H18

Coupled-wire constructions: New insights into the physics of interacting topological systems in two and three dimension (and beyond) — •Tobias Meng[1], Eran Sela[2], Titus Neupert[3], Martin Greiter[4], Ronny Thomale[4], Adolfo G. Grushin[5], Jens H. Bardarson[5], and Kirill Stengel[6] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Tel Aviv 69978, Israel — [3]Princeton Center for Theoretical Science, Princeton University, Princeton, New Jersey 08544, USA — [4]Institute for Theoretical Physics, University of Würzburg, 97074 Würzburg, Germany — [5]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany. — [6]Department of Physics & Astronomy, University of California, Riverside, California 92521, USA

Recently, it has been shown that coupled-wire constructions (CWCs) reproduce well-known fractional quantum Hall phases, and allow to derive new insights into, and setups for, interacting topological systems. I will review the basic concepts of 2D CWCs, discuss how they can teach us about spontaneous time-reversal symmetry breaking in topological insulators, and how they can be used to engineer chiral spin liquids in arrays of Mott-gapped quantum wires. I will show that 3D CWCs can for instance describe Weyl semimetals, and finally present new results on 4D fractional quantum Hall states built from coupled wires, whose 3D edges support a fractional chiral metal with a fractional chiral anomaly, thus generalizing the Weyl semimetal.

TT 32.2 Tue 14:30 H18

Revealing puddles of electrons and holes in compensated topological insulators — •Nick Borgwardt[1], Jonathan Lux[2], Zhiwei Wang[1,3], Ignacio Vergara[1], Malte Langenbach[1], Achim Rosch[2], Yoichi Ando[1,3], Paul van Loosdrecht[1], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für theoretische Physik, Universität zu Köln — [3]Institute of Scientific and Industrial Research, Osaka University

Three-dimensional topological insulators harbour metallic surface states with exotic properties. In transport or optics, these properties are typically masked by defect-induced bulk carriers. Compensation of donors and acceptors reduces the carrier density, but the bulk resistivity remains disappointingly small. We show that measurements of the optical conductivity in $BiSbTeSe_2$ pinpoint the presence of electron-hole puddles in the bulk at low temperatures, which is essential for understanding DC bulk transport. The puddles arise from large fluctuations of the Coulomb potential of donors and acceptors, even in the case of full compensation. Surprisingly, the number of carriers appearing within puddles drops rapidly with increasing temperature and almost vanishes around 40 K. Monte Carlo simulations show that a highly non-linear screening effect arising from thermally activated carriers destroys the puddles at a temperature scale set by the Coulomb interaction between neighbouring dopants, explaining the experimental observation semi-quantitatively [1].

[1] N. Borgwardt et al., arXiv:1508.03212

TT 32.3 Tue 14:45 H18

Interaction Correction to the Magneto-Electric Polarizability of Z_2 Topological Insulators — •Karin Everschor-Sitte[1], Matthias Sitte[1], and Allan MacDonald[2] — [1]Institut für Physik - Johannes Gutenberg-Universität Mainz, Deutschland — [2]Department of Physics - University of Texas at Austin, USA

When time-reversal symmetry is weakly broken and interactions are neglected, the surface of a Z_2 topological insulator supports a half-quantized Hall conductivity $\sigma_S = e^2/(2h)$. A surface Hall conductivity in an insulator is equivalent to a bulk magneto-electric polarizability, *i.e.* to a magnetic field dependent charge polarization. By performing an explicit calculation for the case in which the surface is approximated by a two-dimensional massive Dirac model and time-reversal symmetry is broken by weak ferromagnetism in the bulk, we demonstrate that

there is a non-universal interaction correction to σ_S. Our prediction can be tested by measuring the capacitance of magnetized thin films in which the anomalous quantum Hall effect is absent.

TT 32.4 Tue 15:00 H18

Electron-Phonon Interaction in Surface States of Topological Insulators from First Principles — •Rolf Heid[1], Irina Yu. Sklyadneva[2], and Eugine V. Chulkov[2] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie — [2]Donostia International Physics Center (DICP), San Sebastian/Donostia, Spain

Transport through the metallic 2D surface states of 3D topological insulators with a Dirac-like dispersion is controlled by many-body interactions. In particular, a large electron-phonon interaction could be a limiting factor for applications at elevated temperatures [1]. Previous experimental investigations of the coupling constant remained inconclusive as they found large variations ranging from <0.1 to 3 [2].

Here we present a first principles investigation of the electron-phonon interaction in surface states of topological insulators within density-functional perturbation theory including spin-orbit interaction [3], using Bi_2Se_3, Bi_2Te_3, and Sb_2Te_2S as prominent examples. We discuss the various challenges faced by this approach, such as the rather deep penetration of the surface state and the small momentum range of both electronic and phonon states relevant for the coupling. We find that the coupling strength exhibits a significant dependence on the binding energy, following essentially the available electronic phase space. We further investigate the variation of the coupling with doping to mimic typical experimental conditions.

[1] D. Kim et al., PRL **109**, 166801 (2012)
[2] X. Zhu et al., arXiv: 1307.4559
[3] R. Heid et al., PRB **81**, 174527 (2010)

TT 32.5 Tue 15:15 H18

Detection of current-induced spin polarization in $BiSbTeSe_2$ toplogical insulator — •Fan Yang[1], Subhamoy Ghatak[1], Alexey Taskin[1], Yuichiro Ando[2], and Yoichi Ando[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]Department of Electronic Science and Engineering, Kyoto University, Japan

Topological insulators (TIs) are a class of quantum matter which possess spin-momentum-locked Dirac Fermions on the surfaces. Due to the spin-momentum locking, spin polarization will be induced when a charge current flows through the surface of a TI. Such spin polarization can be detected by using a ferromagnetic tunneling contact as a detector. In this talk, we present our results measured in devices fabricated from $BiSbTeSe_2$ flakes. Spin signals were observed in both n-type and p-type $BiSbTeSe_2$ samples.

TT 32.6 Tue 15:30 H18

Transport measurements on epitaxial $Bi_{1-x}Sb_x$ thin films grown on Si(111) — •Julian Koch, Philipp Kröger, Herbert Pfnür, and Christoph Tegenkamp — Leibniz Universität Hannover, Inst. für Festkörperphysik, Appelstr. 2, 30167 Hannover

The alloy $Bi_{1-x}Sb_x$ can be tuned to be either topologically trivial or non-trivial by changing the relative concentrations of Bismuth and Antimony [1]. In this study we present surface transport measurements performed on non-trivial $Bi_{1-x}Sb_x$ films. Thin films grown by in-situ co-deposition on Si(111) substrates are used, in order to reduce bulk contributions and to provide the possibility of nanostructuring. The morphology was controlled by low energy electron diffraction. Temperature dependent transport measurements for temperatures from 12 to 300 K were performed for films of different stoichiometry ranging from $x = 0.14 - 0.22$ and thicknesses of 4, 8, 16 and 24 nm. We find strong evidence for metallic surface transport in addition to activated bulk transport, which is, to the best of our knowledge, the first observation of metallic surface transport in $Bi_{1-x}Sb_x$ films. In previous studies the transport findings were discussed solely in terms of impurity and bulk bands (see e.g. [2]). For films thinner than 6 nm the surface transport is strongly suppressed, in accordance with measurements on Bi_2Se_3 [3]. The temperature dependent transport behaviour of these films is similar to that of thicker films with substracted surface contribution as well as to films examined in previous studies, further supporting the observation of metallic surface transport in thicker films.

[1] H. Guo, K. Sugawara, A. Takayama, S. Souma, T. Sato, N. Satoh, A. Ohnishi, M. Kitaura, M. Sasaki, Q.-K. Xue, and T. Takahashi, PRB **83**, 201104(R)
[2] S. Cho, A. DiVenere, G. K. Wong, J. B. Ketterson, and J. R. Meyer, PRB **59** 10691
[3] A. A. Taskin, S. Sasaki, K. Segawa, and Y. Ando, PRL **109**, 066803

TT 33: Superconductivity: Cryodedetectors & Cryotechnique

Time: Tuesday 14:00–15:30 Location: H19

TT 33.1 Tue 14:00 H19

Performance and readout of state-of-the-art MMC detector arrays — •M. Wegner, D. Hengstler, J. Geist, M. Keller, M. Krantz, C. Schötz, S. Kempf, L. Gastaldo, A. Fleischmann, and C. Enss — Kirchhoff-Institute for Physics, Heidelberg University

Metallic magnetic calorimeters (MMCs) are energy dispersive particle detectors which have a very good energy resolution, a large dynamic range as well as an excellent linearity. An MMC operates at millikelvin temperatures and converts the energy of an incoming particle into a rise of temperature of an absorber and an attached paramagnetic temperature sensor. The resulting change of sensor magnetization is read out by a SQUID and serves as a measure for the energy input.

One of our goals is the development of large detector arrays to provide a large detection area for low-rate applications, to cope with a significantly increased count rate or to provide imaging capabilities. For this, we have developed several medium-scale detector arrays which are optimized for x-rays up to 20, 30 and 200 keV, respectively. They have a resolving power $E/\Delta E$ above 1500 and are read out using individual dc-SQUIDs. To account for the readout of very large arrays with up to 1000 detectors, we develop a cryogenic frequency domain multiplexer which enables the readout of such large arrays using only one HEMT amplifier and two coaxial cables.

In this contribution we present our micro fabricated detector arrays and discuss their performance in the field of high resolution X-ray spectroscopy. In addition we show for the very first time a simultaneous readout of MMCs using our cryogenic multiplexer.

TT 33.2 Tue 14:15 H19

A 4k-pixel molecule camera for position and energy resolving detection of neutral molecular fragments — •Dennis Schulz[1], Andreas Fleischmann[1], Lisa Gamer[1], Loredana Gastaldo[1], Sebastian Kempf[1], Claude Krantz[2], Oldřich Novotný[2], Andreas Wolf[2], and Christian Enss[1] — [1]Kirchhoff Institute for Physics, Heidelberg — [2]Max Planck Institute for Nuclear Physics, Heidelberg

Stored beams of molecular ions at kinetic energies of some tens or hundreds of keV are widely used in molecular collision physics, and a mass spectroscopic identification of fragmentation products is often a key requirement for unambiguous data interpretation. For the reconstruction of the kinematics of electron-ion collisions at the Cryogenic Storage Ring (CSR, MPIK Heidelberg) we developed MOCCA, a new large-area 4096-pixel detector based on magnetic micro-calorimeters. Here, the kinetic energy deposited by a fragmented reaction product in one of the pixels is a measure of its mass, as all fragments have roughly the speed of the initial molecular ion. This calorimetric approach allows for identification of all fragments, in particular including neutrals. MOCCA has an active area of 45mm x 45mm, which is segmented into 64 x 64 absorbers, each 700μm x 700μm in size.

We discuss design considerations and present micro-fabricated detectors. We discuss the results of first tests with x-ray photons, including the uniformity of the detector response, cross-talk, multi-hit capability and the energy resolution for photons and for the massive particles. Including all effects, we expect MOCCA to easily resolve mass differences down to $1u$ for molecules with a few hundred mass units at CSR.

TT 33.3 Tue 14:30 H19

Low-frequency excess flux noise in superconducting devices — •Sebastian Kempf, Anna Ferring, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Heidelberg, Germany.

Low-frequency noise is a rather universal phenomenon and appears in physical, chemical, biological or even economical systems. However,

there is often very little known about the underlying processes leading to its occurrence. In particular, the origin of low-frequency excess flux noise in superconducting devices has been an unresolved puzzle for many decades. Its existence limits, for example, the coherence time of superconducting quantum bits or makes high-precision measurements of low-frequency signals using SQUIDs rather challenging. Recent experiments suggest that low-frequency excess flux noise in Josephson junction based devices might be caused by the random reversal of interacting spins in surface layer oxides and in the superconductor-substrate interface. Even if it turns out to be generally correct, the underlying physical processes, i.e. the origin of these spins, their physical nature as well as the interaction mechanisms, have not been resolved so far.

In this contribution we discuss recent measurements of low-frequency SQUID noise which we performed to investigate the origin of low-frequency excess flux noise in superconducting devices. Within this context we give an overview of our measurement techniques and link our data with present theoretical models and literature data.

TT 33.4 Tue 14:45 H19

Fluorescence Measurements and Perspectives with Superconducting Tunneling Junctions (STJ) — •Ivan Baev[1], Jan-Hendrik Rüscher[1], Jens Viefhaus[2], Michael Martins[1], and Wilfried Wurth[1,2] — [1]Physics Department, University of Hamburg — [2]DESY Photon Science, Hamburg

The use of STJ's as absorber material for spectroscopic Soft X-Ray detection is very promising in terms of energy resolution and count rate capabilities. Because of the low excitation energy of Cooper pairs in a superconductor (few meV) three orders of magnitude more charge carriers than in a Si-detector are produced per photon. The ultimate resolution limit for such a detector is therefore in the order of a few eV instead of a few 100 eV in the soft X-ray regime. The first commercially available 36 pixel STJ detector is characterized and implemented into synchrotron radiation beamline operation. The achieved resolution is 10eV for 500 eV photons and 50eV for 1500eV photons with a maximal count rate of 10 kcps per pixel. This allowed for element specific Soft X-Ray fluorescence measurements at the P04 beamline at Petra III, DESY.

TT 33.5 Tue 15:00 H19

A large array of silicon microcalorimeters for storage ring experiments — •Saskia Kraft-Bermuth[1], Victor Andrianov[2], and Pascal Scholz[1] — [1]Justus-Liebig-Universität, Gießen, Germany — [2]Lomonosov Moscow State University, Moscow, Russia

Silicon microcalorimeters have already demonstrated the potential to considerably improve the experimental accuracy for X-ray experiments at heavy ion storage rings. To improve their performance with respect to statistical as well as systematic uncertainties, a large array of silicon microcalorimeters for high-precision X-ray spectroscopy, especially optimized for experiments at storage rings, has now been designed. In particular, the large dynamic range will allow the intrinsic determination of the Doppler correction, which is a prominent source of systematic uncertainty in such experiments. The contribution will present the design of the new detector array as well as the readout and data acquisition system. In addition, vibration studies of the cryogen-free dilution refrigerator will be presented.

TT 33.6 Tue 15:15 H19

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

The operation of superconducting optical sensors requires low-noise cooling techniques at temperatures down to 4-5 K, but only needs cooling powers well below 100 mW. Because of the rising l-He prices and even temporary shortage, cryogen-free cooling systems become more and more attractive. Among such dry cooling systems, PTCs, when compared to Stirling- and GM-cryocoolers, have an advantage due to the absence of a cold moving displacer. This unique feature leads to a low level of mechanical vibrations, lower EMI, and increased reliability of the cold head. While there are 4 K GM-type PTCs today that operate with a 2 kW helium-compressor and deliver a cooling power of about 250 mW at 4.2 K, we are developing an even smaller two-stage PTC within the framework of the BMBF joint project SUSY for cooling of bolometers and SNSPDs at temperatures near 5 K. The new PTC has an input power of less than 1 kW to reduce the intrinsic vibrations and improve the temperature stability. Numerical simulations of this new PTC show that it will, despite its small size and input power, still provide enough cooling power to operate the sensors.

Work supported by the German BMBF under grant no. 13N13444

TT 34: Correlated Electrons: Frustrated Magnets - Chiral Magnets & $RuCl_3$

Time: Tuesday 14:00–16:00 Location: H20

TT 34.1 Tue 14:00 H20

Experimental determination of the Fermi surface in the itinerant helimagnet MnSi — Matthias Dodenhöft[1], •Schorsch Michael Sauther[1], Stephan Gerhard Albert[1], Felix Rucker[2], Andreas Bauer[2], Marc Andreas Wilde[1], Christian Pfleiderer[1,2], and Dirk Grundler[1,3] — [1]Phys.-Dep. E10, TU München — [2]Phys.-Dep. E51, TU München — [3]LMGN, IMX, STI, EPF Lausanne

Manganese silicide (MnSi) is an itinerant helimagnet that has been studied for over five decades. Its cubic crystal structure lacks inversion symmetry. The strong electronic correlations in MnSi result in a rich phase diagram with a helimagnetic ground state. Further, MnSi is the material in which the topologically exotic skyrmion lattice phase has been discovered [1]. This triggered a large interest. However, a thorough experimental determination of the Fermi surface (FS) of bulk MnSi is still lacking. In our experiment, we employ torque magnetometry at low temperatures T and in high magnetic fields B to measure the magnetization M of high-quality, single-crystalline bulk samples of MnSi. We observe quantum oscillations in $M(B)$, i.e. the de Haas-van Alphen effect, with multiple frequencies which correspond to extremal cross sections of the FS. We study the angular dependence of these oscillations and extract the effective electron masses from the temperature dependence of the oscillation amplitudes. The experimental findings are compared to the FS calculated via density functional theory.

[1] S. Mühlbauer *et al.*, Science **323**, 915 (2009)

TT 34.2 Tue 14:15 H20

Uniaxial pressure dependence of magnetic order in MnSi — •Alfonso Chacon[1], Andreas Bauer[1], Tim Adams[1], Felix Rucker[1], Georg Brandl[1,2], Robert Georgii[1,2], Markus Garst[3], and Christian Pfleiderer[1] — [1]Physik Department, Technische Universität München, James-Franck-Strasse 1, 85748 Garching, Germany — [2]Heinz Maier Leibnitz (MLZ), Technische Universität München, Lichtenbergstr., D-85748 Garching, Germany — [3]Institute for Theoretical Physics, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany

We report the ac susceptibility and small angle neutron scattering (SANS) of the helical order, conical phase and skyrmion lattice phase (SLP) in MnSi under uniaxial pressures. For all crystallographic orientations uniaxial pressure imposes a strong easy-axis anisotropy along the pressure axis on the modulation direction . In turn, under applied magnetic fields uniaxial pressure favours the magnetic order for which a magnetic modulation is closest to the pressure axis. In particular, uniaxial pressures perpendicular to the magnetic field axis enhance the SLP strongly on the expense of the conical phase, whereas the SLP is suppressed for pressure parallel to the field. Yet, for both orientations key characteristics of the SANS pattern of the SLP remain essentially unaffected. Our results establish how strain allows to control skyrmions in chiral magnets.

TT 34.3 Tue 14:30 H20

The microscopic NMR probe in chiral magnets: zero field-, field-modulated- and Skyrmion- states in FeGe and MnSi — •Michael Baenitz[1], Hiroshi Yasuoka[1], Mayukh Majumder[1], Panchanan Khuntia[1], Sebastian Witt[2], Cornelius Krellner[2],

and Markus Schmidt[1] — [1]MPI for the Chemical Physics of Solids, 01187 Dresden, Germany — [2]Goethe University Frankfurt, 60438 Frankfurt am Main, Germany

Cubic FeGe is a prototype B20 chiral magnet (T_c = 280 K) which allows to study chiral correlations directly "on-site" via the^{57}Fe nucleus because of its S=1/2 nuclear spin interacting only with the electron spin moment. NMR provides the static and dynamic staggered local magnetization M_Q through the hyperfine field (H_{hf}) and the spin lattice relaxation rate (SLRR = $1/T_1$). Measurements were performed on randomly oriented ^{57}Fe enriched FeGe single crystals between 2-300 K. Helical- , conical- and field-polarized-states could be clearly identified and spin dynamics of each phase was investigated. MnSi single crystals and ^{29}Si enriched MnSi polycrystals were studied by ^{29}Si-NMR (S=1/2) in the ordered state (T_c = 29 K) and above. The T- and H- dependence of H_{hf} and SLRR was investigated in great detail for both FeGe and MnSi.The ^{29}Si-NMR lines in MnSi are narrow and H_{hf}-values obtained are smaller than in FeGe. Our results are in general accordance with the extended SCR theory for itinerant helical magnets [1], although the theory does not include the symmetry breaking in the B20 structure and the multi-band nature. For FeGe correlations are complex due to its more localized magnetism.

[1] T. Moriya, J. Phys. Soc. Jpn. **40**, 933 (1976)

TT 34.4 Tue 14:45 H20

Magnon spectrum of the helimagnetic insulator Cu_2OSeO_3 — P. Y. Portnichenko[1], J. Romhányi[2], Y. A. Onykiienko[1], A. Henschel[3], M. Schmidt[3], A. S. Cameron[1], M. A. Surmach[1], J. A. Lim[1], J. T. Park[4], A. Schneidewind[5], D. L. Abernathy[6], H. Rosner[3], J. van den Brink[7], and •D. S. Inosov[1] — [1]TU Dresden — [2]MPI-FKF, Stuttgart — [3]MPI-CPfS, Dresden — [4]MLZ, Garching — [5]JCNS, Jülich — [6]ORNL, Oak Ridge — [7]IFW Dresden

Complex low-temperature ordered states in chiral magnets are typically governed by a competition between multiple magnetic interactions. The chiral-lattice multiferroic Cu_2OSeO_3 became the first insulating helimagnetic material in which a long-range order of topologically stable spin vortices known as skyrmions was established. We employed state-of-the-art inelastic neutron scattering (INS) to comprehend the full three-dimensional spin excitation spectrum of Cu_2OSeO_3 over a broad range of energies. Distinct types of high- and low-energy dispersive magnon modes separated by an extensive energy gap are observed in excellent agreement with the previously suggested microscopic theory based on a model of entangled Cu_4 tetrahedra. The comparison of our INS data with model spin-dynamical calculations based on these theoretical proposals enables an accurate quantitative verification of the fundamental magnetic interactions in Cu_2OSeO_3 that are essential for understanding its abundant low-temperature magnetically ordered phases.

TT 34.5 Tue 15:00 H20

Critical dynamics in $LiCuVO_4$ — •Christoph Grams[1], Petra Becker[2], and Joachim Hemberger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Kristallographie, Universität zu Köln, Germany

Without an external magnetic field the 1D spin chain compound $LiCuVO_4$ has a phase transition into a cycloidal spin ordered phase below $T_N = 2.3$ K where it simultaneously is antiferromagnetic and ferroelectric. The transition temperature of this phase transition can be lowered with increasing magnetic field. Ferroelectric phase transitions are of continuous type and are accompanied by a symmetry lowering that yields soft modes. Near the critical point the dynamics show a "critical slowing down" scenario.

We studied the magnetic field and temperature dependence of $\varepsilon(\nu)$ in $LiCuVO_4$ in the vicinity of the multiferroic phase transition by means of broadband dielectric spectroscopy. While we find the expected relaxational behavior close to T_N, below 0.4 K a nearly gapless excitation is observed as was theoretically predicted in terms of chiral solitons [1].

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

[1] S. Furukawa *et al.*, JPSJ **77**, 123712 (2008)

TT 34.6 Tue 15:15 H20

High-frequency ESR studies and the magnetic phase diagram of chiral-structured $MnSb_2O_6$ — •Johannes Werner[1], Changhyun Koo[1], Elena Zvereva[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Faculty of Physics, Moscow State University, Moscow, Russia

Magnetic properties of the chiral-structured magnet $MnSb_2O_6$ ($P321$ phase) were investigated by means of static magnetization and high-frequency electron-spin-resonance (HF-ESR) studies. The ground state has been reported to exhibit incommensurate order based on corotating cycloids [1]. Our studies confirm T_N = 11.5 K but imply at least three different AFM phases appearing in the magnetic phase diagram. HF-ESR spectra of the $MnSb_2O_6$ powder sample at frequencies of f $\sim$ 260 GHz and f $\sim$ 38 GHz show a single resonance feature at high temperatures, respectively, which significantly broadens upon cooling. In addition, the resonance shifts to lower fields when temperature is approaching T_N, signaling the evolution of local fields. At low-temperatures, the magnetic field vs. frequency diagram exhibits two resonance branches which are associated with the antiferromagnetic resonance (AFMR) modes. The AFMR branches are linear in the range of 70 GHz to 320 GHz but the low field resonance branch shows an upturn indicating a zero-field splitting of ZFS = 22 GHz. The data are analyzed in terms of an AFMR mean field model with six sublattices.

[1] R. D. Johnson, K. Cao, L. C. Chapon, F. Fabrizi, N. Perks, P. Manuel, J. J. Yang, Y. S. Oh, S.-W. Cheong, P. G. Radaelli, PRL **111**, 017202 (2013).

TT 34.7 Tue 15:30 H20

Thermal conductivity of a 2D honeycomb material — •Richard Hentrich[1], Keerthi Dorai Swamy Reddy[1], Bernd Büchner[1], Maximilian Geyer[1], Anja Wolter-Giraud[1], Jennifer Sears[2], Young-June Kim[2], Domenic Nowak[3], Anna Isaeva[3], Thomas Doert[3], and Christian Hess[1] — [1]IFW Dresden, Germany — [2]Department of Physics, University of Toronto, Canada — [3]Inorganic Chemistry Department II, Dresden University of Technology, Germany

α-$RuCl_3$ is a material composed of hexagonal layers of edge sharing $RuCl_6$ octahedra in a $J_{\text{eff}} = 1/2$ state due to a combination of Coulomb repulsion and strong spin orbit coupling. This kind of spin structure is a possible realisation of the Heisenberg-Kitaev model for which theory predicts a multitude of non-trivial excitations. Thermal transport measurements are known as a valuable tool to probe elementary excitations of systems with low dimensional spin structure. We have investigated transport properties of α-$RuCl_3$ single crystals and found an anomalous behaviour of the heat conductivity parallel to the honeycomb planes. The clear deviation from a purely phononic signal suggests that additional excitations are contributing to heat transport.

TT 34.8 Tue 15:45 H20

Magnetic and Thermodynamic Characterisation of α-$RuCl_3$ — •Maximilian Geyer[1], Laura Theresa Corredor Bohorquez[1], Sebastian Gass[1], Wolf Schottenhamel[1], Anja Wolter-Giraud[1], Anna Isaeva[2], Domenic Nowak[2], Thomas Doert[2], and Bernd Büchner[1,2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Technische Universität Dresden, Helmholtzstraße 10, 01069 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. Particulary α-$RuCl_3$ seems to be a suitable candidate for the experimental realisation of the Kitaev-Model due to its $J_{eff} = 1/2$ state and its layered honeycomb lattice of Ru^{3+} ions in the $4d^5$ configuration. This leads to highly anisotropic magnetic properties in this compound . We report on specific heat and magnetisation measurements for α-$RuCl_3$ single crystals grown by means of chemical transport reactions. Furthermore magnetisation experiments under high pressure were conducted on this compound.

TT 35: Correlated Electrons: Quantum-Critical Phenomena - Theory

Time: Tuesday 14:00–15:45 Location: H21

TT 35.1 Tue 14:00 H21

Thermal phase transitions in the vicinity of the quantum critical point of spinless fermions on the honeycomb lattice — •Stephan Hesselmann and Stefan Wessel — Institute for Theoretical Solid State Physics, JARA-FIT, and JARA-HPC, RWTH Aachen University, 52056 Aachen, Germany

We consider spinless fermions on a honeycomb lattice (spinless $t-V$ model), which provide a minimal realization of lattice Dirac fermions. Nearest neighbor interactions drive a quantum phase transition from a semi-metallic phase to a charge ordered phase, which spontaneously breaks the chiral Z_2 symmetry of the Dirac fermions. The critical theory is given by the Gross-Neveu-Yukawa theory, which describes the process of mass generation due to the broken chiral symmetry. At finite temperature (and $V > V_c$) the quantum critical point connects to a line of second order thermal phase transitions that restore the broken chiral symmetry. We employ a recent sign-problem-free continuous time quantum Monte Carlo method [1, 2] to investigate the finite temperature phase diagram of the model. Furthermore we give estimates for the critical exponents of the Gross-Neveu chiral Ising universality class by studying the extension of the quantum critical regime to finite temperatures.

[1] E. F. Huffman et al., PRB **89**, 111101(R) (2014)
[2] L. Wang et al., New J. Phys. **16**, 103008 (2014)

TT 35.2 Tue 14:15 H21

Monte Carlo study of competing orders in a nearly antiferromagnetic metal — •Max Henner Gerlach[1], Yoni Schattner[2], Simon Trebst[1], and Erez Berg[2] — [1]Institute for Theoretical Physics, University of Cologne, Cologne, Germany — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel

We study the onset of antiferromagnetism in itinerant electron systems via a two-dimensional lattice model amenable to sign-problem-free determinantal quantum Monte Carlo simulations. These numerically exact simulations allow to precisely determine not only the boundaries of the magnetic phase, but also a dome-shaped d-wave superconducting phase near the putative antiferromagnetic quantum critical point. We discuss the entire phase diagram of this 2D model with regard to antiferromagnetic, superconducting, charge density wave, and pair density wave susceptibilities, as well as the superfluid density. We further find fluctuation diamagnetism well above the superconducting T_c and demonstrate where the electronic density of states displays the opening of a gap. Our results provide insights into the interplay of antiferromagnetism and unconventional superconductivity at intermediate to strong coupling.

TT 35.3 Tue 14:30 H21

Spin trimers coupled in 2D — •Dominik Strassel and Sebastian Eggert — Department of Physics and Research Center Optimas, University Kaiserslautern, 67663 Kaiserslautern, Germany

We study linear clusters of three strongly coupled $\mathcal{S} = \frac{1}{2}$ spins (trimers), which are weakly connected in a two dimensional lattice. For this we use Stochastic Series Expansion Quantum Monte Carlo simulations of the Heisenberg model in a magnetic field. These systems show a magnetization plateau at $\frac{1}{3}$ saturation, which is already known from strongly coupled three-leg ladders. In contrast to the frustrated triangular lattice which also shows a $\frac{1}{3}$ plateau, our systems do not suffer from the infamous minus sign problem. With increasing coupling between the trimers the plateau vanishes and a bi-critical point can be identified. To understand this in more detail we develop an effective two boson model describing these systems analytically, which allows us to calculate the behavior near the bi-critical point (e.g. magnetization).

TT 35.4 Tue 14:45 H21

Excitonic instability of three-dimensional gapless semiconductors with quadratic Fermi node — •Lukas Janssen[1,2] and Igor F. Herbut[2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, Germany — [2]Department of Physics, Simon Fraser University, Burnaby, Canada

Three-dimensional gapless semiconductors with quadratic band touching, such as HgTe, α-Sn, or the pyrochlore iridate $Pr_2Ir_2O_7$, are believed to display a non-Fermi-liquid ground state due to long-range electron-electron interaction. I will argue that this state is inherently unstable towards spontaneous formation of a (topological) excitonic insulator. The instability can be parameterized by a critical fermion number N_c, in formal analogy to the problem of mass generation in (2+1)-dimensional quantum electrodynamics (QED_{2+1}). For $N < N_c$ the rotational symmetry is spontaneously broken, the system develops a gap in the spectrum, and features a finite nematic order parameter. To the leading order in the $1/N$ expansion and in the static approximation, the analogy with QED_{2+1} yields $N_c = 16/[3\pi(\pi-2)]$. Taking the important dynamical screening effects into account, we find that $N_c \geq 2.6(2)$, and therefore safely above the physical value of $N = 1$. I will also discuss results of recent complementary approaches to the problem using $2+\epsilon$ expansion and functional renormalization group, respectively, which turn out to arrive at a similar conclusion. Some experimental consequences of the nematic ground state will be pointed out.

[1] L. Janssen and I. F. Herbut, arXiv:1509.01737 [cond-mat.str-el]

TT 35.5 Tue 15:00 H21

Violation of hyperscaling at the Ising-nematic quantum critical point in a two-dimensional metal — •Andreas Eberlein[1], Ipsita Mandal[2], and Subir Sachdev[1,2] — [1]Department of Physics, Harvard University, Cambridge, USA — [2]Perimeter Institute for Theoretical Physics, Waterloo, Canada

Spatially isotropic critical quantum states in d spatial dimensions which have the hyperscaling property have an optical conductivity that scales as $\omega^{(d-2)/z}$ for high frequencies $\omega >> T$, where T is the temperature and z the dynamic critical exponent. We examine the Ising-nematic quantum critical point in $d = 2$ using the fixed point theory[1] and compute the optical conductivity in an expansion in $\epsilon = 5/2 - d$. We show that hyperscaling is violated at this quantum critical point and discuss the scaling behaviour of the optical conductivity at $T = 0$.

[1] Dalidovich and Lee, PRB **88**, 245106 (2013)

TT 35.6 Tue 15:15 H21

Dimensionless ratios: characteristics of quantum liquids and their phase transitions — Yi-Cong Yu[1], Yang-Yang Chen[1], Hai-Qing Lin[2], •Rudolf A. Römer[3], and Xi-Wen Guan[1,4,5] — [1]Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, China — [2]Beijing Computational Science Research Center, Beijing 100094, China — [3]University of Warwick, Coventry, CV4 7AL, UK — [4]Center for Cold Atom Physics, Chinese Academy of Sciences, Wuhan 430071, China — [5]Australian National University, Canberra ACT 0200, Australia

Dimensionless ratios of physical properties can be constant in low-temperatures phases in a wide variety of materials. As such, the Wilson ratio (WR), the Kadowaki-Woods ratio and the Wiedemann-Franz law capture essential features of Fermi liquids in metals, heavy fermions, etc. Here we prove that the phases of many-body interacting multi-component quantum liquids in one dimension can be described by WRs based on the compressibility, susceptibility and specific heat associated with each component. These WRs arise due to surprisingly simple additivity rules within subsystems reminiscent of the rules for multi-resistor networks in series and parallel. Using experimentally realized multi-species cold atomic gases as examples, we prove that the Wilson ratios uniquely identify phases of Tomonaga-Luttinger liquids, while providing universal scaling relations at the boundaries between phases. Their values within a phase identify the internal degrees of freedom of said phase such as its spin-degeneracy.

TT 35.7 Tue 15:30 H21

Many-body localization from one particle density matrix — •Soumya Bera[1], Henning Schomerus[2], Fabian Heidrich-Meisner[3], and Jens Bardarson[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Lancaster University, Lancaster, United Kingdom — [3]Ludwig-Maximilians-Universitaet Munchen, Munich, Germany

We show that the one-particle density matrix ρ can be used to characterize the interaction-driven many-body localization transition in isolated fermionic systems. The natural orbitals (the eigenstates) are localized in the many-body localized phase and spread out when one

enters the delocalized phase, while the occupation spectrum (the set of eigenvalues) reveals the distinctive Fock- space structure of the many-body eigenstates, exhibiting a step-like discontinuity in the localized phase. The associated one-particle occupation entropy is small in the localized phase and large in the delocalized phase, with diverging fluctuations at the transition.

TT 36: Transport: Quantum Coherence and Quantum Information Systems - Theory 2 (Joint session of HL, MA and TT organized by TT)

Time: Tuesday 14:00–15:00 Location: H22

TT 36.1 Tue 14:00 H22

Emulating the 1-Dimensional Fermi-Hubbard Model with Superconducting Qubits — •Jan-Michael Reiner, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

A chain of qubits with both ZZ and XX couplings is described by a Hamiltonian which coincides with the Fermi-Hubbard model in one dimension. The qubit system can thus be used to study the quantum properties of this model. We investigate the specific implementation of such an analog quantum simulator by a chain of tunable Transmon qubits, where the ZZ interaction arises due to an inductive coupling and the XX interaction due to a capacitive coupling.

TT 36.2 Tue 14:15 H22

A method to efficiently simulate the thermodynamic properties of the Fermi-Hubbard model on a quantum computer — •Pierre-Luc Dallaire-Demers and Frank K. Wilhelm — Saarland University, Saarbrücken, Germany

Many phenomena of strongly correlated materials are encapsulated in the Fermi-Hubbard model whose thermodynamic properties can be computed from its grand canonical potential. In general, there is no closed form expression of the grand canonical potential for lattices of more than one spatial dimension, but solutions can be numerically approximated using cluster methods. To model long-range effects such as order parameters, a powerful method to compute the cluster's Green's function consists in finding its self-energy through a variational principle. This allows the possibility of studying various phase transitions at finite temperature in the Fermi-Hubbard model. However, a classical cluster solver quickly hits an exponential wall in the memory (or computation time) required to store the computation variables. Here it is shown theoretically that the cluster solver can be mapped to a subroutine on a quantum computer whose quantum memory usage scales linearly with the number of orbitals in the simulated cluster and the number of measurements scales quadratically. A quantum computer with a few tens of qubits could therefore simulate the thermodynamic properties of complex fermionic lattices inaccessible to classical supercomputers.

TT 36.3 Tue 14:30 H22

Scattering of photons on Bose-Hubbard lattices — •Kim Georg Lind Pedersen and Mikhail Pletyukhov — Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen

We study the photonic transport of weakly coherent light in various Bose-Hubbard lattice geometries implemented as QED cavity arrays. We use a diagrammatic scattering approach to study the relation between lattice geometry and the second order intensity correlation of the transmitted light. The motivation is twofold: First, a large induced correlation can be used to design circuit elements useful for "photonics applications". Second, the scattering of photons on complex lattices offers a promising way to characterize quantum correlation in a range of different, exotic states of matter theorized to be present in higher-dimensional cavity arrays.

TT 36.4 Tue 14:45 H22

Quantum Simulation of Hawking Radiation With Surface Acoustic Waves — •Raphael Schmit, Bruno G. Taketani, and Frank K. Wilhelm — Saarland University, Theoretical Physics Departement

In 1975, Hawking predicted particles and light to leave the surface of a black hole. This so called Hawking radiation follows the thermal spectrum of a black body with a certain temperature, called Hawking temperature. Its investigation is extremely desired since scientists believe it to provide clues for unanswered questions like the trans-Planckian problem or the information paradox, but a direct observation is challenging since the Hawking temperature is too small or the distance to the black hole is too large. For this purpose, we propose an experimental setup for emulating a black hole and measuring its analogue Hawking radiation. The setup consists of two adjacent piezoelectric semiconducting layers, one of them carrying a flying qubit serving as detector for Hawking radiation, and the other one with an attached MOS diode structure, imposing an effective curved metric on the surface acoustic wave (SAW) propagation. In the moving reference frame of the flying qubit, this metric matches the Painlevé-Gullstrand-metric describing an uncharged, non-rotating black hole with an event horizon for SAWs. We show that for GaAs as used layer material, the system can possess Hawking radiation in the μK regime. The flying qubit interacts with the Hawking phonons via piezoelectrically induced photons, and thus can be used to measure the temperature of the Hawking phonons.

TT 37: Transport: Fluctuation and Noise (Joint session of DY and TT organized by TT)

Time: Tuesday 14:00–15:45 Location: H23

TT 37.1 Tue 14:00 H23

Super-Poissonian shot noise of squeezed-magnon mediated spin transport — •Akashdeep Kamra and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

The magnetization of a ferromagnet (F) driven out of equilibrium injects pure spin current into an adjacent conductor (N). Such F|N bilayers have become basic building blocks in a wide variety of spin based devices. We evaluate the shot noise of the spin current traversing the F|N interface when F is subjected to a coherent microwave drive. We find that the noise spectrum is frequency independent up to the drive frequency, and increases linearly with frequency thereafter. The low frequency noise indicates super-Poissonian spin transfer understood in terms of dipolar interaction mediated squeezing of F eigenmodes, which results in quasi-particles with effective spin $\hbar^* = \hbar(1+\delta)$. For experimentally relevant parameters, we estimate $\delta \approx 0.4$ for yttrium iron garnet and $\delta \approx 3.0$ for iron thin films. The spontaneous squeezing of F eigenmodes suggests novel possibilities for their applications in quantum optics and related fields.

TT 37.2 Tue 14:15 H23

Statistics of transmission eigenvalues in diffusive star-shaped multi-terminal structures — •Sven Essert, Viktor Krueckl, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We study transport in diffusive star-shaped devices with more than two leads. We find that the eigenvalue distribution $p(t)$ of the transmission matrix between any pair of terminals is typically not showing the bimodal distribution that is found in two-lead devices. Instead, the distribution displays a cutoff t_c, i. e., $p(t) = 0$ for $1 \geq t \geq t_c$. We

explain the origin of this cutoff by deriving analytical expressions in the limit of low transmission for fully symmetric stars and for some limiting cases of extreme asymmetry. Using numerical calculations we probe the validity of these results away from the low-transmission limit.

In addition, we note that the bimodal distribution can be recovered when combining the leads of the star into meta leads in such a way that the total number of such meta leads is two. Then the transport between these is again bimodal, thus showing "open channels" with transmissions close to 1. Related to this, we propose the study of a new observable, which we call eigenvector splitting, that quantifies the distribution of outgoing flux among the constituent leads of the meta lead. This quantity becomes particularly interesting, when studying devices in the low-transmission limit, where it directly relates to the eigenvalue distribution. We present analytical solutions for the eigenvector splitting in some limiting geometries and supplement them by numerical calculations.

TT 37.3 Tue 14:30 H23

Detection of interactions via generalized factorial cumulants in systems in and out of equilibrium — •Philipp Stegmann[1], Björn Sothmann[2], Alfred Hucht[1], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [2]Départment de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

We introduce time-dependent, generalized factorial cumulants $C_s^m(t)$ of the full counting statistics of electron transfer as a tool to detect interactions in nanostructures [1]. The violation of the sign criterion $(-1)^{m-1}C_s^m(t) \geq 0$ for *any* time t, order m, and parameter s proves the presence of interactions. For given system parameters, there is a minimal time span $t_{\min}$ and a minimal order m to observe the violation of the sign criterion. We demonstrate that generalized factorial cumulants are more sensitive to interactions than ordinary ones [2, 3] and can detect interactions even in regimes where ordinary factorial cumulants fail. We illustrate our findings with the example of a quantum dot tunnel coupled to electronic reservoirs either in or out of equilibrium.

[1] P. Stegmann, B. Sothmann, A. Hucht, and J. König, PRB **92**, 155413 (2015)
[2] D. Kambly, C. Flindt, and M. Büttiker, PRB **83**, 075432 (2011)
[3] D. Kambly and C. Flindt, J. Comput. Electron. **12**, 331 (2013)

TT 37.4 Tue 14:45 H23

Time-resolved statistics of entangled photon pairs in Josephson photonics — •Simon Dambach, Björn Kubala, and Joachim Ankerhold — Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany

The interplay of the tunneling transfer of charges and the emission and absorption of light can be investigated in a setup where a voltage-biased Josephson junction is placed in series to a microwave resonator. Such circuits combine phenomena and observational tools originally known from the fields of charge transfer physics and quantum optics (Josephson photonics). Due to the inherent nonlinearity of the Josephson junction, tunneling Cooper pairs can create a variety of nonclassical states of light. This is reflected in form of characteristic signatures in the second-order correlation function $g^{(2)}(\tau)$ and the waiting-time distribution $w(\tau)$. We find that this device represents a versatile source of nonconventional light which can be tuned from photon-pair creation and strong bunching to single-photon creation and complete antibunching [1].

In this talk, we will investigate theoretically the simultaneous creation of two photons within different modes and, in particular, address the question of intermode entanglement by means of different entanglement witnesses.

[1] S. Dambach et al., PRB **92**, 054508 (2015).

Invited Talk TT 37.5 Tue 15:00 H23

Dynamical Coulomb Blockade theory of resonantly enhanced light emission from a tunnel junction — •Wolfgang Belzig[1], Fei Xu[1], and Cecilia Holmqvist[2] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

Inelastic tunneling of electrons generates emission of photons, whose energies intuitively should be limited by the applied bias voltage. However, experiments indicate that more complex processes involving the interaction of electrons with plasmon polaritons lead to photon emission characterized by over-bias energies. We have proposed a model of this observation [1] in analogy to the dynamical Coulomb blockade, originally developed for treating the electronic environment in mesoscopic circuits, and explained the experimental finding quantitatively by the correlated tunnelling of two electrons interacting with an LRC circuit modelling the local plasmon-polariton mode. Furthermore, we calculate the over-bias emission at finite temperature and discuss the possibility of non-classical light emission.

[1] F. Xu, C. Holmqvist, W. Belzig, PRL **113**, 066801 (2014).

TT 37.6 Tue 15:30 H23

Correlations of weak quantum measurements in a non-Markovian detection scheme — •Johannes Bülte[1], Adam Bednorz[2], Christoph Bruder[3], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Faculty of Physics, University of Warsaw, PL02-093 Warsaw, Poland — [3]Department of Physics, University of Basel, CH-4056 Basel, Switzerland

Generalized quantum measurement schemes are described by positive operator-valued measures that go beyond the projection postulate, i.e., the instantaneous collapse of the systems' wave function by the measurement. They allow to consider the noninvasive limit of so-called weak measurements, and, in particular, to investigate the correlations of several such measurements which permits the tracking of noncommuting observables. We propose a scheme in which the detectors are coupled to the measured system for a finite time which leads to non-Markovian effects [1]. We derive microscopic expressions for the memory functions which are related to the Kubo linear-response formalism. The deviations from the standard Markovian measurement with symmetrized operator order (Keldysh ordering) can be traced back to a detector-detector interaction mediated by the measured system. Finally, we discuss different detector types, and show that an appropriate choice enables e.g. the proof of the non-classical nature of a system by second-order correlation functions.

[1] A. Bednorz, C. Bruder, B. Reulet, and W. Belzig, PRL **110**, 250404 (2013)

TT 38: Frontiers of Electronic Structure Theory: Focus on Topology and Transport I (Joint session of DS, HL, MA, MM, O and TT organized by O)

Time: Tuesday 14:00–16:00 Location: H24

Topical Talk TT 38.1 Tue 14:00 H24

Topological semimetals and chiral transport in inversion asymmetric systems — •Shuichi Murakami — Department of Physics and TIES, Tokyo Institute of Technology, Tokyo, Japan

Weyl semimetals (WS) are semimetals with nondegenerate 3D Dirac cones in the bulk. We showed that in a transition between different Z2 topological phases, the Weyl semimetal phase necessarily appears when inversion symmetry is broken. In the presentation we show that this scenario holds for materials with any space groups without inversion symmetry. Namely, if the gap of an inversion-asymmetric system is closed by a change of an external parameter, the system runs either into (i) a Weyl semimetal phase or (ii) a nodal-line semimetal, but no insulator-to-insulator transition happens. This transition is realized for example in tellurium (Te). Tellurium has a unique lattice structure, consisting of helical chains, and therefore lacks inversion and mirror symmetries. At high pressure the band gap of Te decreases and finally it runs into a Weyl semimetal phase, as confirmed by our ab initio calculation. We also theoretically propose chiral transport in systems with such helical structures.

TT 38.2 Tue 14:30 H24

Topological orbital magnetic moments — •Manuel dos Santos

Dias, Juba Bouaziz, Mohammed Bouhassoune, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Orbital magnetic moments are usually associated with the spin-orbit interaction (SOI). We explore from first-principles how topological orbital magnetic moments (TOMs) can emerge in non-trivial magnetic spin textures, even without SOI, justifying the 'topological' label. Firstly, the case of magnetic trimers on the Cu(111) surface illustrates the basic symmetry properties of the TOMs, and how to separate their contribution from the usual SOI-driven orbital moments. We then focus on the implications of TOMs for single magnetic skyrmions formed in Pd/Fe/Ir(111) [1], considering their possible use in detecting and distinguishing skyrmions from anti-skyrmions by optical means.

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

[1] D.M. Crum et al., Nat. Comms. **6**, 8541 (2015)

TT 38.3 Tue 14:45 H24

The orbital Rashba effect — •Dongwook Go[1,2], Patrick Buhl[1], Gustav Bihlmayer[1], Yuriy Mokrousov[1], Hyun-Woo Lee[2], and Stefan Blügel[1] — [1]Institute for Advanced Simulation and Peter Grünberg Institut, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Department of Physics, Pohang University of Science and Technology, 37673 Pohang, Korea

We present a new surface phenomenon called the *orbital* Rashba effect, analogous to the spin Rashba effect. The effect is described by the orbital Rashba Hamiltonian, $H_{\text{orb-R}}(\mathbf{k}) = \alpha_{\text{orb-R}}\mathbf{L}\cdot(\hat{\mathbf{z}}\times\mathbf{k})$, where $\mathbf{L}$ is the orbital moment derived from atomic orbitals and $\alpha_{\text{orb-R}}$ is the orbital Rashba constant. This leads to orbital-dependent energy splittings and orbital texture in the $\mathbf{k}$-space. The mechanism behind the emergence of the $H_{\text{orb-R}}(\mathbf{k})$ can be understood as the $\mathbf{k}$-dependent magnetoelectric coupling due to atomic orbital hybridization. In the presence of intra-atomic spin-orbit coupling, the spin moment is aligned parallel or antiparallel to the orbital moment, thus the spin Rashba effect is recovered. As an example, we present a tight-binding and an *ab initio* study of the Bi/Ag(111) surface alloy, where the hybridization between a Ag *s*-orbital and a Bi *p*-orbital leads to the orbital Rasbha effect that is dominant over the spin one. The orbital Rashba effect is a key to new physics and to understanding spin-orbit driven physics at surfaces and interfaces, such as Dzyaloshinskii-Moriya interaction, non-collinear magnetism, etc.

TT 38.4 Tue 15:00 H24

Spin and orbital magnetism of Rashba electrons induced by magnetic nanostructures — •Juba Bouaziz, Manuel dos Santos Dias, Phivos Mavropoulos, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We explore theoretically the spin and orbital magnetism of Rashba electrons in the presence of noncollinear impurity-induced magnetic states. The Rashba electron gas mediates the Dzyaloshinksii-Moriya interaction between magnetic impurities favoring chiral states [1]. Here we investigate the back-action of such noncollinear magnetic states on the Rashba electron gas. The presence and distribution of ground state spin and orbital currents is analyzed. Surprisingly, when switching off the spin-orbit coupling, chiral magnetic textures generate bound currents, which implies the existence of orbital magnetic moments originating solely from the peculiar topology of the impurities magnetic moments. In the particular case of a single adatom with an out of plane magnetic moment, we found circular currents flowing around the magnetic impurity in agreement with the continuity equation for the electric charge. Similar results were predicted for magnetic adatoms on superconductor surfaces with a finite spin-orbit coupling [2].

[1] J. Bouaziz *et al.* in preparation.
[2] S. S. Pershoguba *et al.* Phys. Rev. Lett. **115**, 116602 (2015).

This work is supported by the HGF-YIG Programme VH-NG-717 (Functional Nanoscale Structure and Probe Simulation Laboratory).

TT 38.5 Tue 15:15 H24

First-principles investigation of the impact of single atomic defects on magnetic skyrmions — •Imara L. Fernandes, Benedikt Schweflinghaus, Juba Bouaziz, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Chiral magnetic skyrmions are topological spin-swirling textures with rich physics and technological potential in the field of information storage. In a device, skyrmions certainly interact with defects and imperfections resulting into pinning phenomena. We explore from first-principles the non-trivial impact of 3d and 4d impurities on the energetics, electronic and magnetic properties of single magnetic skyrmions. Utilizing the newly developed Jülich full-potential relativistic Korringa-Kohn-Rostoker Green function method [1], we focus on topological magnetic objects of sub-5nm diameters stabilized in a single ferromagnetic layer of Fe sandwiched between the Ir(111) surface and one or two Pd layers, where the tunneling spin-mixing magnetoresistance (TXMR) was demonstrated theoretically [2] and experimentally [3]. – Funding provided by the HGF-YIG Program VH-NG-717 and the CNPq (BRAZIL).

[1] D. S. G. Bauer, Schriften des Forschungszentrum, Key Tech. **79** (2014).
[2] D.M. Crum *et al.*, Nat. Comms. **6**, 8541 (2015).
[3] C. Hanneken *et al.*, Nat. Nanotech. Doi:10.1038/nano.2015.218 (2015).

TT 38.6 Tue 15:30 H24

Topological magnons: Any chance to find them? — •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

Topological magnon insulators (TMIs) have a nontrivial topology due to the Dzyaloshinskii-Moriya interaction which results in spatially confined edge states and, thus, energy and spin currents along their edges [1,2]. Several systems have been identified as TMIs, for example, Cu(1,3-benzenedicarboxylate) consisting of kagome planes [3], or the family of ferromagnetic pyrochlore oxides, e. g., $Lu_2V_2O_7$, showing the magnon Hall effect [4]. However, to date, no direct experimental evidence of a topological magnon band has been provided, what comes down to the small total width of the magnon dispersion relation and the energy resolution of surface sensitive measurements.

We propose Fe_3Sn_2 as promising candidate for a TMI. The total width of its magnon dispersion relation is large, and we determine its nontrivial topology by constructing an effective spin Hamiltonian. On this basis, we discuss signatures of topological magnon states that should be looked for in experiments.

[1] L. Zhang et al., PRB **87**, 144101 (2013); [2] A. Mook et al., Phys. Rev. B **89**, 134409 (2014); *eidem*, Phys. Rev. B **90**, 024412 (2014); *eidem*, Phys. Rev. B **91**, 224411 (2015); *eidem*, Phys. Rev. B **91**, 174409 (2015); [3] R. Chisnell et al., Phys. Rev. Lett. **115**, 147201 (2015); [4] Y. Onose et al., Science **329**, 297 (2010).

TT 38.7 Tue 15:45 H24

Acoustic magnons in the long-wavelength limit: resolving the Goldstone violation in many-body perturbation theory — •Mathias C.T.D. Müller, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Ferromagnetic materials exhibit a spontaneously broken global rotation symmetry in spin space leading to the appearance of massless quasiparticles (zero gap) in the long-wavelength limit. These magnons are formed by the correlated motion of electron-hole pairs with opposite spins, which we describe from first principles employing the T-matrix formalism in the ladder approximation within the FLAPW method [1]. Due to approximations used in the numerical scheme, the acoustic magnon dispersion exhibits a small but finite gap at Γ. We analyze this violation of the Goldstone mode and present an approach that implements the magnetic susceptibility using a renormalized Green function instead of the Kohn-Sham (KS) one. This much more expensive approach shows substantial improvement of the Goldstone-mode condition. In addition, we discuss a possible correction scheme, that involves an adjustment of the KS exchange splitting, which is motivated by the spin-wave solution of the one-band Hubbard model. The new exchange splittings turn out to be closer to experiment. We present corrected magnon spectra for the elementary ferromagnets Fe, Co, and Ni.

[1] E. Şaşıoğlu *et al.*, Phys. Rev. B **81**, 054434 (2010); C. Friedrich *et al.* Top. Curr. Chem. **347**, 259 (2014).

TT 39: Spintronics
(Joint session of DS, HL, MA, O and TT organized by O)

Time: Tuesday 14:00–16:00 Location: S051

TT 39.1 Tue 14:00 S051

Skyrmion à la carte: Engineering magnetic skyrmions at transition-metal multilayers — •Bertrand Dupé[1], Gustav Bihlmayer[2], Marie Böttcher[1], Stefan Blügel[2], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel, 24098 Kiel, Germany — [2]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Due to their unique topological and dynamical properties skyrmions in magnetic materials offer attractive perspectives for future spintronic applications [1]. Recently, it has been discovered that magnetic skyrmions can also occur in ultra-thin transition metal films at surfaces [2,3]. However, so far only skyrmions at interfaces with a single atomic layer of a magnetic material were reported, which greatly limits their potential for application in devices. Here, we predict the emergence of skyrmions in $[4d/Fe_2/5d]_n$ multilayers, i.e. structures composed of Fe biatomic layers sandwiched between 4*d*- and 5*d*-transition-metal layers [4]. In these composite structures, the exchange and the Dzyaloshinskii-Moriya interactions, which control skyrmion formation, can be tuned separately by the two interfaces. This allows engineering skyrmions as shown by density functional theory and spin dynamics simulations. [1] A. Fert, *et al.*, Nature Nano. **8**, 152 (2013). [2] N. Romming, *et al.*, Science **341**, 636 (2013). [3] B. Dupé, *et al.*, Nature Comm. **5**, 4030 (2014). [4] B. Dupé, *et al.*, submitted (arXiv :1503.08098).

TT 39.2 Tue 14:15 S051

Multichannel-Spin-Polarimetry for the Analysis of Spin-Transport in Metal-Organic Interfaces — •Erik Schaefer[1,2], Martin Krämer[1], Dmytro Kutnyakhov[1], Katerina Medjanik[1], Gerd Schönhense[1,2], and Hans-Joachim Elmers[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz — [2]Graduate School Materials Science in Mainz, Mainz

Spin- and angular resolved photoemission spectroscopy has become the key technique for the investigation of electronic properties of promising spintronic materials. In contrast to conventional photon optics, an effective spin polarization analysis of a given electron beam is difficult. Since organic materials tend to degrade within a short period, a massive reduction of spin-resolved data acquisition time is crucial. The recent developed multichannel spin- and angle-resolved photoemission spectroscopy [1] solves this issue by enhancing the figure of merit by several orders of magnitudes. Ir(001) shows high potential for the use as a scattering target in multichannel spin analysis [2]. A new Ir(001) multichannel spin-detection system was constructed and the important quantities and efficiency of the system were determined. Spin- and angle-resolved photoemission spectroscopy of thin iron films on W(110) were performed.

Founded by Stiftung Rheinland Pfalz für Innovation (project 1038)

[1] M. Kolbe et al., Phys. Rev. Lett. 107, 207601 (2011)
[2] D. Kutnyakhov et al., Ultramicroscopy 130, 63-69 (2013)

TT 39.3 Tue 14:30 S051

Spin-resolved ToF momentum-microscopy of anomalous surface states on W(110) — •D. Kutnyakhov[1], S.V. Chernov[1], R. Wallauer[1], K. Medjanik[2], S.A. Nepijko[1], C. Tusche[3], M. Ellguth[3], S. Borek[4], J. Braun[4], J. Minár[4,5], H. Ebert[4], H.J. Elmers[1], and G. Schönhense[1] — [1]Institut für Physik, Uni-Mainz — [2]MAX IV Lab., Lund, Sweden — [3]MPI für Mikrostrukturphysik, Halle — [4]Dep. Chemie, LMU München — [5]University of West Bohemia, Pilsen, Czech Republic

Spin-resolved bandmapping of anomalous surface states on W(110) has been performed via time-of-flight (ToF) momentum microscopy with an imaging spin-filter using synchrotron radiation at the beamline U125-NIM at BESSY II ($h\nu$=22 eV). 3D (k_x,k_y,E_B)-maps in the full surface Brillouin zone with 3.4 $Å^{-1}$ dia. and 4 eV binding energy range were measured simultaneously, resolving 2.5×10^5 voxels without and more than 10^4 voxels with spin resolution. Similar to our recent experiment on Mo(110) [1] the results give evidence for d-like surface resonances in the spin-orbit induced partial band gap. In agreement with previous results [2], we find the dispersing state with Dirac-like signature and Rashba spin texture crossing the bandgap at the $\overline{\Gamma}$-point and E_B=1.25 eV. A second linear band crossing occurs close to the midpoint between $\overline{\Gamma}$ and $\overline{N}$ at E_B=0.8 eV. Results are compared with one-step photoemission calculations in its density matrix formulation.

Funded by BMBF (05K13UM1, 05K12EF1, 05K13WMA). [1] Chernov et al., Ultramicroscopy, (2015), doi:10.1016/j.ultramic.2015.07.008; [2] Miyamoto et al., PRL 108, 066808 (2012)

TT 39.4 Tue 14:45 S051

Spin-polarized electron energy loss spectrometer with detection of final state spin polarization — •Dmitry Vasilyev and Jürgen Kirschner — Max-Planck Institut für Mikrostrukturphysik, Halle, Germany

Spin polarized electron energy loss spectroscopy (SPEELS) allows to investigate Stoner excitations, as was demonstrated 30 years ago. Based on theory one should expect structured energy loss spectra with features on the scale of less than 1 eV. The spectra should change with varying the incidence angle by a few degrees, and the primary energy of electrons by less than 1 eV. However, this was not observed at that time. We have developed a new SPEELS apparatus with the detection of final state spin polarization. The new spectrometer allows us to see all the expected features. Spin-polarized electrons are generated via photoemission from GaAs-based superlattice. The direction of the electron spin can be changed by varying the light helicity. Additionally the magnetization of the target can be reversed. A multichannel spin detector is used for the measurement of the spin-polarization of the outgoing electrons. It is based on spin dependent reflection from pseudomorphic Au on Ir (001). This system provides high polarization sensitivity, up to 80%, and more that 8 months lifetime in ultrahigh vacuum. The measurement of intensity asymmetries for opposite magnetization directions allows to distinguish between spin-orbit asymmetry and exchange asymmetry. Together with detection of the spin-polarization of the outgoing electrons it allows to determine relative transition probabilities for each of the four partial intensities.

TT 39.5 Tue 15:00 S051

Ab initio investigation of a novel spin-filter: Graphene on Ir(111) — •Christian Mende[1], Stephan Borek[1], Jürgen Braun[1], Gustav Bihlmayer[2], Dima Kutnyakhov[3], Hans-Joachim Elmers[3], Gerd Schönhense[3], Jan Minár[1,4], and Hubert Ebert[1] — [1]Ludwig-Maximilians-Universität München — [2]Forschungzentrum Jülich — [3]Johannes-Gutenberg-Universität Mainz — [4]University of West Bohemia Pilsen

For the determination of the spin-polarized band structure in angle-resolved photoemission (ARPES) experiments an application of materials as reflection mirrors is recommended. For this purpose one uses the spin-dependent scattering of photoelectrons from suitable surfaces based on either exchange or spin-orbit induced scattering. We present our calculations of spin-polarized low energy electron diffraction (SPLEED) patterns for the clean Ir(111) and the Graphene covered Ir(111) surface. For these materials the electron scattering is strongly influenced by spin-orbit interaction whereas the Graphene layer provides a longer lifetime of the spin-polarizing mirror due to its inert properties concerning surface contamination. Based on ab initio calculations of the electronic structure we obtained diffraction patterns over a wide range of kinetic energies and polar angles to determine the applicability of the Ir(111)+Graphene system as spin-polarizing mirror. Additionally we investigated ARPES spectra to connect the electronic structure calculations to the corresponding experiment.

TT 39.6 Tue 15:15 S051

Ab initio calculation of SPLEED patterns for the Ir(111) surface — •Stephan Borek[1], Jürgen Braun[1], Jan Minár[1,2], Dima Kutnyakhov[3], Hans-Joachim Elmers[3], Gerd Schönhense[3], and Hubert Ebert[1] — [1]Ludwig-Maximilians-Universität München — [2]University of West Bohemia Pilsen — [3]Johannes-Gutenberg-Universität Mainz

Recent investigations have shown that the Ir(100) surface is a promising candidate for spin-filter application [1]. In our studies we investigated the Ir(111) surface and its applicability for spin-filter purposes. Accordingly, diffraction patterns of spin-polarized electrons scattered on the surface have been calculated for a wide range of polar angles and

kinetic energies. The calculated diffraction patterns show more suitable working points in comparison to the standard Ir(100) surface extending the spin-filter versatility. In addition we looked for deviations of the scattering plane from high symmetry directions $\overline{\Gamma}\,\overline{M}$ and $\overline{\Gamma}\,\overline{K}$ in the surface Brillouin zone and its impact on the diffraction patterns. To complement the SPLEED calculations we calculated angle-resolved photoemission spectra to characterize the underlying electronic structure.

[1] D. Kutnyakhov et al. Ultramicroscopy **130**, 63 (2013)

TT 39.7 Tue 15:30 S051

Determining excitation pathways at the Cobalt/Alq3 interface — •Philip Thielen[1,2], Anna-Katharina Mahro[1], Benjamin Stadtmüller[1], Mirko Cinchetti[1], and Martin Aeschlimann[1] — [1]Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Gottlieb-Daimler-Str. 47, 67663 Kaiserslautern, Germany

One of the fundamental questions in molecular spintronics consists in understanding the properties of hybrid interfaces between molecules and ferromagnetic metals. Recently, it was shown that the interface state between a thin layer of the metalorganic complex tris(8-hydroxyquinolinato)aluminium (Alq3) and a cobalt surface acts as a spin filter due to the prolonged spin-dependent trapping of electrons [1]. The excitation of spin-polarized electrons into such hybrid interface states can take place either directly from the cobalt in a coherent process or in an indirect, incoherent process, e.g. via charge transfer. We show that we can disentangle coherent and incoherent excitation pathways using a phase-stabilized two-pulse correlation experiment. We discuss the possible implications of our findings regarding the optical control of spin-polarized electrons at hybrid interfaces.

References: [1] S. Steil, N. Großmann, M. Laux, A. Ruffing, D. Steil, M. Wiesenmayer, S. Mathias, O. L. A. Monti, M. Cinchetti and M. Aeschlimann, Nature Physics 9, 242 - 274 (2013)

TT 39.8 Tue 15:45 S051

Energy Dispersion and Spin Structure of Unoccupied States of BiTeI: A Matter of Surface Termination? — •Christian Langenkämper[1], Koji Miyamoto[1], Anke B. Schmidt[1], Peter Krüger[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Germany

We present a combined experimental and theoretical study on the unoccupied electronic structure of BiTeI along the $\overline{\Gamma}$-$\overline{\mathrm{K}}$ direction. We performed spin-resolved inverse-photoemission experiments on samples with different surface termination, Te and I.

For the two surface terminations we found distinct differences in the energy dispersion of the surface states around $\overline{\Gamma}$, which are caused by band bending. In contrast, this effect is not observed around the $\overline{\mathrm{K}}$ point. With the help of *ab initio* band-structure calculations we identify the observed states as bulk states, not influenced by band bending.

In addition, we studied the spin structure of the unoccupied bands. Around the $\overline{\Gamma}$ point, we found a Rashba-type in-plane spin polarization. Upon approaching $\overline{\mathrm{K}}$, the direction of the spin polarization rotates from fully in-plane to out-of-plane. This spin texture is in accordance with the crystal symmetry and independent of the surface termination.

TT 40: Graphene: Optics (Joint session of DS, DY, HL, MA, O and TT organized by HL)

Time: Tuesday 14:45–15:45 Location: H17

Invited Talk TT 40.1 Tue 14:45 H17

Ultrafast carrier dynamics in monolayer graphene — •Daniele Brida — Department of Physics and Center for Applied Photonics, University of Konstanz, Universitätsstr. 10, D-78464 Konstanz, Germany

The impulsive optical excitation of carriers in graphene creates an nonequilibrium distribution, which thermalizes on an ultrafast timescale. The hot Fermi-Dirac distribution subsequently cools via phonon emission within few hundreds of femtoseconds. We investigated the initial stages of the thermalization process that are dominated by electron-electron scattering events. By comparing the two-color pump-probe experimental data with different models, that solve the quantum Boltzmann equation by implementing three different screening methods, we can visualize the importance of Auger recombination processes, such as carrier multiplication, in the ultrafast relaxation of the electronic distribution along the Dirac cone in graphene. Recent theoretical and experimental work also emphasizes the role of the polarization state of the light pulses used for the excitation. When carriers are excited with linearly polarized light, the resulting occupation in momentum space is not isotropic due to the pseudospin selection rules. To observe this anisotropy we compare the transient absorption signal arising for probe pulses with polarizations parallel and perpendicular to the pump pulse. We identify electron-phonon scattering as main driving mechanism of isotropization of the electronic distribution across the Dirac cone since it occurs in approximately 100 fs.

TT 40.2 Tue 15:15 H17

Noncollinear Coulomb scattering in graphene — •Jacob C. König-Otto[1,2], Martin Mittendorff[3], Torben Winzer[4], Ermin Malic[5], Andreas Knorr[4], 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]University of Maryland, USA — [4]Technische Universität Berlin, Germany — [5]Chalmers University of Technology, Sweden

Utilizing the anisotropy of the optical excitation in graphene, we reveal the twofold nature of Coulomb scattering in graphene. The initial nonequilibrium charge carrier distribution in graphene created by linearly polarized light possesses a pronounced anisotropy, which has been observed in our recent experiment [1]. In the present study we perform polarization-dependent pump-probe measurements using a photon energy of 88 meV to suppress efficiently the optical phonon scattering. In this case the relaxation dynamics leading to an isotropic distribution is dominated by noncollinear Coulomb scattering. By varying the pump fluence over a range of several orders of magnitudes we are able to successfully control the efficiency of this process. This reveals a surprising twofold nature of Coulomb scattering in graphene: Whereas collinear Coulomb scattering is known to be a very fast process on the fs timescale, noncollinear scattering is remarkably slow, resulting in a thermalization time of several ps in our experiment. Our experimental findings are complemented by the results of microscopic modelling.

[1] M. Mittendorff et al., Nano Lett. **14**, 1504 (2014).

TT 40.3 Tue 15:30 H17

Gate-Voltage Dependency of Förster Transfer in Graphene - Quantum Dot Photo Detection — •Lorenz Maximilian Schneider[1], Ruifeng Li[2], Huizhen Wu[2], Martin Koch[1], and Arash Rahimi-Iman[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Department of Physics and the State Key Laboratory of Silicon Materials, Zhejiang University, Hangzhou, 310058, P.R. China

Graphene photodetectors functionalized by colloidal Quantum dots (cQDs) have been recently demonstrated for effective photo detection. Nevertheless, the transfer of the energy or charge carriers from cQDs to graphene is not sufficiently understood. Here, we present a respective study of a graphene field-effect transistor, which is functionalized with CdSe/ZnS Core-Shell QDs covering it's conductive channel. In order to investigate energy transfer dynamics in this system, we have investigated the time-resolved photo-luminescence from the cQDs as function of the applied gate voltage. A clear change in the photo-luminescence lifetime has been observed, indicating a change of the decay channels. In support of our findings, we provide data for a Förster-like energy transfer model as a function of the gate voltage. The model shows that by applying a backgate voltage to the photo detector, absorbance can be tuned with respect to the photo-luminescence of the cQDs, changing the energy transfer rate of the photo-detector.

TT 41: Symposium Topological Insulators: Status Quo and Future Directions (SYTI) (Joint symposium of HL, MA, O and TT organized by TT)

Time: Wednesday 9:30–13:00 Location: H1

Invited Talk TT 41.1 Wed 9:30 H1

Topological insulators and topological superconductors — •Shoucheng Zhang — Dept of Physics, Stanford University

In this talk, I will first give a brief overview on topological insulators and superconductors. I will then discuss the recent theoretical prediction and the experimental observation of the quantum anomalous Hall effect in magnetic topological insulators. I shall present a newly predicted material called stanene, and discuss its potential applications.

Invited Talk TT 41.2 Wed 10:10 H1

Three-dimensional topological insulators and superconductors — •Yoichi Ando — II. Physikalisches Institut, Universität zu Köln

A topological quantum state of matter is characterized by a nontrivial topological structure of its Hilbert space. 3D topological insulators are characterized by non-trivial Z_2 topology, which is due to band inversion caused by strong spin-orbit coupling [1]. Intriguingly, when superconductivity shows up upon doping charge carriers into 3D topological insulators, the resulting superconducting state can also be topological [2], because the strong spin-orbit coupling could lead to an unconventional gap function characterized by a new Z_2 topological invariant [3]. In this talk, I will present experimental realizations of these materials and report recent efforts to address their exotic properties.

[1] Y. Ando, J. Phys. Soc. Jpn. **81**, 102001 (2013)
[2] Y. Ando and L. Fu, Ann. Rev. Cond. Mat Phys. **6**, 361 (2015)
[3] S. Sasaki, M. Kriener, K. Segawa, K. Yada, Y. Tanaka, M. Sato, and Y. Ando, PRL **107**, 217001 (2011)

Invited Talk TT 41.3 Wed 10:50 H1

Interplay of magnetic and electronic states in pyrochlore iridates — •Leon Balents — University of California, Santa Barbara, CA, USA

The pyrochlore iridates are a series of compounds undergoing antiferromagnetic ordering and metal-insulator transitions. They are of interest because they combine electron correlation effects and the potential for non-trivial band topology. We will discuss the theoretical picture of these materials, from electronic structure to magnetism and phase transitions, and how they may be controlled through applied fields and temperature. Comparison will be made between theory and recent experiments.

10 min. break

Invited Talk TT 41.4 Wed 11:40 H1

Magnetic imaging of edge states — •Kathryn Moler — Stanford University

Beautiful theoretical proposals launched the field of topological materials, followed rapidly by great initial successes in synthesizing and demonstrating several topological insulators. The challenges now are to understand and control edge and surface scattering, to find materials with no bulk states and large gaps for high-temperature operation, and most importantly, to fabricate integrated devices that include gates, superconductors, and ferromagnets. Scanning SQUID microscopy can aid this effort by imaging magnetism, superconductivity, and current flow. Images of current flow in two quantum spin hall insulators verify that currents really do flow on the edges, provide images of the developing edge states with voltage and temperature, and also help reveal the conditions for achieving topological vs. trivial edge states. Sensitive magnetic measurements characterize superconductor * topological insulator structures, and help to determine the conditions for achieving exotic Josephson junctions.

Invited Talk TT 41.5 Wed 12:20 H1

Sub-nm wide edge states at the dark side of a weak topological insulator — •Markus Morgenstern — II. Institute of Physics B and JARA-FIT, RWTH Aachen, 52074 Aachen

Three-dimensional insulating crystals, which respect time reversal symmetry, can be classified as trivial insulators, strong topological insulators and weak topological insulators (WTIs). Many examples of trivial or strong topological insulators are known, but WTIs have barely been probed. They offer pairs of topologically protected surface states on most surfaces, but exhibit one dark surface without such surface states. The step edges of this dark surface naturally belong to the bright surfaces such that they contain spin helical edge states with perfect e^2/h conductivity. The first WTI $Bi_{14}Rh_3I_9$ was synthesized recently [1]. Here, we show by scanning tunneling spectroscopy that the edge states indeed exist and are below 1 nm wide. They can be scratched into the surface using an atomic force microscope providing a simple tool to guide them [2]. Moreover, it is shown that the edge state can be removed by chemically dimerizing adjacent layers of the WTI. Strategies to bring the edge state to the Fermi level are discussed.

[1] B. Rasche, A. Isaeva, M. Ruck, S. Borisenko, V. Zabolotnyy, B. Büchner, K. Koepernik, C. Ortix, M. Richter, and J. van den Brink, Nature Mater. **12**, 422 (2012)
[2] C. Pauly, B. Rasche, K. Koepernik, M. Liebmann, M. Pratzer, M. Richter, J. Kellner, M. Eschbach, B. Kaufmann, L. Plucinski, C. M. Schneider, M. Ruck, J. van den Brink, and M. Morgenstern, Nature Phys. **11**, 338 (2015)

TT 42: Correlated Electrons: Frustrated Magnets - Cu-based Systems & FeCr

Time: Wednesday 9:30–13:00 Location: H18

TT 42.1 Wed 9:30 H18

Interplay of Spin and Lattice in a Pseudo-Kagome System — Vladimir Gnezdilov[1,2], •Peter Lemmens[2], Yurii Pashkevich[3], Alexander Vasiliev[4], and Peter Berdonosov[4] — [1]ILTPE, Kharkov, Ukraine — [2]IPKM, TU-BS, Braunschweig — [3]DonFTI, Donetsk, Ukraine — [4]MSU, Moskow, Russia

The layered cuprates, francisites $Cu_3Bi(SeO_3)_2O_2X$, with X=Br or Cl, with pseudo-kagome structure were studied across the structural and magnetic phase transitions using Raman spectroscopy. For X=Cl a soft optical mode is revealed. The temperature-dependent changes in the phononic and magnetic subsystems of these highly frustrated magnets allow proposing a microscopic magnetic model including Dzyaloshinsky-Moriya interaction to explain the nature of the observed spin-wave excitations.

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

TT 42.2 Wed 9:45 H18

Peculiarities of structural distortions in kagome francisites — •Alexander A. Tsirlin[1], Danil Prishchenko[2], Vladimir Tsurkan[3], and Vladimir G. Mazurenko[2] — [1]EP VI, Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Ural Federal University, Ekaterinburg, Russia — [3]EP V, Electronic Correlations and Magnetism, University of Augsburg, Germany

Francisites $Cu_3Bi(SeO_3)_2O_2X$ (X = Cl, Br) are spin-$\frac{1}{2}$ kagome materials with predominantly ferromagnetic exchange couplings. Despite this tendency toward ferromagnetism, they entail strong magnetic frustration related to antiferromagnetic couplings between next-nearest neighbors. The infinite classical degeneracy of the ground state is lifted by anisotropic Dzyaloshinsky-Moriya couplings that stabilize canted magnetic order within the kagome planes. The canting angle θ reveals strong dependence on the halogen atom, chlorine ($\theta \simeq 70°$) or bromine ($\theta = 52°$), which is difficult to rationalize assuming that these ions are not part of the kagome planes and have no influence on relevant superexchange couplings. By combining high-resolution synchrotron x-ray diffraction with *ab initio* calculations of lattice dynamics, we show that the Cl francisite undergoes a structural phase transition

triggered by the weakly bonded Cl ions located between the kagome planes. This transition has strong impact on the in-plane magnetism and alters magnetic interactions considerably. In the Br francisite, no structural phase transition is observed, and a more regular version of the kagome lattice is formed.

TT 42.3 Wed 10:00 H18

Substitutions in Cu-based frustrated spin-systems: $BaCuSi_2O_6$ and $ZnCu_3(OH)_6Cl_2$ — •Pascal Puphal[1], Denis Sheptyakov[2], Natalija Van Well[2], Raivo Stern[3], Lars Postulka[1], Bernd Wolf[1], Michael Lang[1], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe Universität Frankfurt, Germany — [2]PSI, Switzerland — [3]National Institute of Chemical Physics and Biophysics, Estonia

$BaCuS_2O_6$ is a spin dimer system presenting a 2D Bose-Einstein condensation of triplons at low temperatures and high magnetic fields. We present a structural analysis of the substituted system $(Ba_{1-x}Sr_x)CuSi_2O_6$, which reveals a stable tetragonal crystal structure down to 2 K unlike its parent compound x = 0. We explore the structural details with low-temperature neutron and synchrotron powder diffraction, room-temperature NMR, as well as magnetic- and specific-heat measurements.

$ZnCu_3(OH)_6Cl_2$ is a highly frustrated kagomé system, which has a antiferromagnetic superexchange interaction of J = 17 meV, but no magnetic transition or long-range order has been observed down to T = 50 mK. We present first results of $M_xCu_{4-x}(OH)_6Cl_2$, with a three valent ion M, which should lead to a Dirac metal as proposed by I. I. Mazin et. al. [1]. We could synthesize a Paratacamite-type (x < 1), which shows a magnetic ordering below 6.5 K. This transition can be decreased with increasing x.

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

TT 42.4 Wed 10:15 H18

Spin model of volborthite $Cu_3V_2O_7(OH)_2{\cdot}2H_2O$ revisited: coupled trimers instead of zigzag chains — •Oleg Janson[1], Shunsuke Furukawa[2], Tsutomu Momoi[3,4], Philippe Sindzingre[5], Johannes Richter[6], and Karsten Held[1] — [1]IFP, TU Wien, Austria — [2]University of Tokyo, Japan — [3]Condensed Matter Theory Laboratory, RIKEN, Japan — [4]RIKEN Center for Emergent Material Science, Japan — [5]Université Pierre & Marie Curie, Paris, France — [6]University of Magdeburg, Germany

Motivated by recent experiments on volborthite single crystals showing a wide $\frac{1}{3}$-magnetization plateau [1], we adopt the structural data and perform microscopic modeling by means of density functional theory (DFT). Using DFT+U, we find four leading magnetic exchanges: antiferromagnetic J and J_2, as well as ferromagnetic J' and J_1. Simulations of the spin Hamiltonian show good agreement with the experiment for $J{:}J'{:}J_1{:}J_2 = 1 : -0.2 : -0.5 : 0.2$ with $J \simeq 252\,\mathrm{K}$. The $\frac{1}{3}$-plateau phase pertains to polarized magnetic trimers formed by strong J bonds. An effective $J \to \infty$ model shows a tendency towards condensation of magnon bound states preceding the plateau phase [2].

[1] H. Ishikawa *et al.*, PRL **114**, 227202 (2015).
[2] O. Janson *et al.*, arXiv:1509.07333.

TT 42.5 Wed 10:30 H18

$Cu_4(OH)_6FBr$ - a structurally perfect spin-1/2 kagome system — •Bernd Wolf[1], Elena Gati[1], Nguyen Hieu Hoang[1], Harald O. Jeschke[2], Francesc Salvat-Pujol[2], Roser Valenti[2], John A. Schleuter[3], and Michael Lang[1] — [1]Physics Institute, Goethe-University Frankfurt(M), Germany, — [2]Institute for Theoretical Physics, Goethe-University Frankfurt(M), Germany, — [3]Division of Materials Research, National Science Foundation, Arlington, Virginia, USA

Spin-1/2 kagome lattices have been intensively investigated in recent years since they support the formation of quantum spin liquids (QSL). A prominent example is the natural mineral herbertsmithite $ZnCu_3(OH)_6Cl_2$ [1]. Here chemical modifications are difficult to realize and therefore new design strategies are necessary for synthesizing novel QSL. $Cu_4(OH)_6FBr$ reflects such a novel approach [2] where a structurally perfect kagome arrangement is achieved. We present a detailed magnetic characterization of small single crystals of $Cu_4(OH)_6FBr$. Measurements of the magnetization and susceptibility down to 2 K and up to 5 T reveal indications for two dominant magnetic couplings of different sign and an antiferromagnetic transition at $T_N = 15$ K exhibiting a weak ferromagnetic component. The experimental findings are in good agreement with the results of density functional theory (DFT) calculations. In addition, we present thermal expansion measurements from which the pressure dependence of T_N is determined.

[1] T.-H. Han et al., Nature **492**, 406 (2012).
[2] H. O. Jeschke et al., PRB **92**, 094417 (2015)

TT 42.6 Wed 10:45 H18

Synthesis and crystal growth of Cu-based kagome materials — •Christian Klein, Franz Ritter, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, D-60438 Frankfurt am Main

Magnetic frustration in kagome-type lattices can lead to novel type of ground states, the so-called Quantum Spin Liquids (QSLs). [1] For studying experimentally the properties of QSLs new materials in single crystalline form are essential.We report on the crystal growth under hydrothermal conditions and characterization of the new material Barlowite ($Cu_4(OH)_6BrF$). [2] Substitution of the cation on the interlayer-site enables us to modify the physical properties. Selective use of non-magnetic ions on the interlayer position leads to a quasi-two-dimensional system by decoupling the exchange between the kagome-layers. [3] We will discuss various synthetic pathways, together with thorough structural characterization.

[1] P. A. Lee, Science **321**, 1306 (2008)
[2] H. Jeschke et al., PRB **92**, 094417 (2015).
[3] Guterding et al., arXiv:1511.05686v1.

TT 42.7 Wed 11:00 H18

Interplay of magnetic sublattices in langite $Cu_4(OH)_6SO_4 \cdot 2H_2O$ — •Satoshi Nishimoto[1,2], Stefan Lebernegg[3], Alexander A. Tsirlin[4], Oleg Janson[5], Günther J. Redhammer[6], Stefan-Ludwig Drechsler[1], and Helge Rosner[3] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]MPI CPfS, Dresden, Germany — [4]Institute of Physics, University of Augsburg, Germany — [5]Institute of Solid State Physics, TU Vienna, Austria — [6]University Salzburg, Austria

Magnetic and crystallographic properties of the mineral langite $Cu_4(OH)_6SO_4 \cdot 2H_2O$ are reported. Density-functional band structure calculations suggest a quasi-two-dimensional spin model consisting of two interacting subsystems: (A) Frustrated Heisenberg chains with ferromagnetic nearest-neighbor (NN) and antiferromagnetic (AFM) next-nearest-neighbor (NNN) exchange couplings, which is responsible for the magnetic ordering at $T_N \simeq 5.7\,\mathrm{K}$, and (B) weakly-coupled frustrated chains with AFM NN and NNN exchange couplings. At low temperature, the magnetic susceptibility of the former subsystem is about five times larger than that of the latter one. Therefore, the system can be regarded as a combination of isolated subsystems with respect to applied magnetic field. The subsystem (A) may give an ideal host exhibiting multipolar physics. Experimentally observed magnetic susceptibility, specific heat, and magnetization are also compared to our numerical results.

15 min. break

TT 42.8 Wed 11:30 H18

Investigation of the antiferromagnetic - ferromagnetic dimer chain compound $BaCu_2V_2O_8$ at zero and finite temperatures — •Ekaterina Klyushina[1,2], Alexander Tiegel[3], Nazmul Islam[1], Jitae Park[4], Bastian Klemke[1], Andreas Honecker[5], Salvatore Manmana[3], and Bella Lake[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [3]Georg-August-Universität Göttingen, Germany — [4]Heinz Maier-Leibnitz Zentrum, TU München, Garching, Germany — [5]Université de Cergy-Pontoise, France

Highly dimerized quantum magnets have attracted a great deal of attention in the recently due to the unconventional temperature behavior of their magnetic excitations[1,2]. Here we present our investigations of the highly dimerized antiferromagnet-ferromagnetic 1D chain $BaCu_2V_2O_8$ both at base and at finite temperatures. The single crystal inelastic neutron scattering measurements at base temperature reveal that there are two excitation branches which disperse along the L direction over the energy range of 36-46 meV. The comparison with DMRG simulations indicates that the antiferromagnetic dimers are coupled ferromagnetically along the c axis. The line shape of the excitations at the dispersion minima was found to become asymmetry with increasing temperature. Thus unconventional thermal behavior also exists in dimer compounds with ferromagnetic interdimer coupling.

[1] D. L. Quintero-Castro et al., PRL **109**, 127206 (2012)
[2] D. Tennant et al., PRB **85**, 014402 (2012).

TT 42.9 Wed 11:45 H18

Neutron diffraction on the frustrated spin-chain linarite at low temperatures and high fields — •Leonie Heinze[1], Britta Willenberg[2], Jens-Uwe Hoffmann[2], Anja U.B. Wolter-Giraud[3], Bernd Büchner[3], Kirrily C. Rule[4], Andrew Studer[4], Bachir Ouladdiaf[5], and Stefan Süllow[1] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig — [2]Helmholtz-Zentrum Berlin für Materialien und Energie — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden — [4]The Bragg Institute, ANSTO — [5]Institut Laue-Langevin Grenoble

The natural mineral linarite, $PbCuSO_4(OH)_2$, has been established as a model compound of the frustrated one-dimensional spin chain with ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor interactions [1]. Recently, it has been demonstrated that it exhibits a complex magnetic phase diagram in applied fields $B \parallel b$ axis up to 9.5 T for temperatures below 2.8 K [2].

Here, we present additional neutron diffraction experiments on the field induced phases of linarite, with special emphasis on the low temperature and high magnetic field regime for fields applied along the crystallographic b axis. This way, the temperature and field dependence of the magnetic moment were established for temperatures down to 50 mK and fields up to 9.5 T. As well, the nature of the phase transitions from phase IV into the surrounding phases being of first order was derived.

[1] B. Willenberg et al., PRL **108** 117202 (2012)
[2] B. Willenberg et al., arXiv:1508.02207

TT 42.10 Wed 12:00 H18

Exotic spin phases in the one-dimensional spin-1/2 quantum magnet $LiCuSbO_4$ as seen by high-field NMR and ESR spectroscopies — •Margarita Iakovleva[1,2,3], Hans-Joachim Grafe[1], Evgeniia Vavilova[3], Vladislav Kataev[1], Alexey Alfonsov[1], Hiroyuki Nojiri[4], Mihai I. Sturza[1], Sabine Wurmehl[1], and Bernd Büchner[1,2] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Zavoisky Physical Technical Institute, Kazan, Russia — [4]Institute of Materials Research, Sendai, Japan

We will present our recent results of high-field NMR and sub-THz ESR studies of the quantum magnet $LiCuSbO_4$ (LCSO) that presents an excellent model system of a one-dimensional spin-1/2 quantum magnet with frustrated exchange interactions. Such networks are predicted to exhibit a plethora of novel ground states beyond classical ferro- or antiferromagnetic phases. In LCSO the absence of a long-range magnetic order down to sub-Kelvin temperatures is suggestive of the realization of a quantum spin liquid state. Our NMR and ESR measurements in strong magnetic fields up to 16 Tesla reveal clear indications for the occurrence of an exotic field-induced hidden phase which we will discuss in terms of multipolar physics.

TT 42.11 Wed 12:15 H18

Theoretical Aspects of Quantum Magnetism in $LiSbCuO_4$ — Satoshi Nishimoto[1], •Stefan-Ludwig Drechsler[1], Ullrich Roessler[1], Roman Kuzian[2], Johannes Richter[3], and Helge Rosner[4] — [1]ITF at the Leibniz Institute IFW-Dresden, 01171 Dresden, Germany — [2]IPMS, Kiev, Ukraine — [3]University of Magdeburg, Germany — [4]MPI-cPfS, Dresden, Dresden

We apply various theoretical methods (DMRG, LDA+U, equation of motion for hard-core bosons, complete diagonalizations, and a full symmetry analysis) to model the recently discovered novel frustrated edge-shared chain cuprate $LiSbCuO_4$ [1] in terms of isotropic and anisotropic interacting J_1-J_1'-J_2 chains including also interchain coupling. Special attention is paid to possible field induced multipolar phases near the saturation field and the remarkable interplay of possible nematicity with symmetric and antisymmetric exchange anisotropy. In particular, the main exchange intra and interchain couplings are estimated, the nature and the role of weak Dzyaloshinskii-Moriya interactions allowed by the low crystal symmetry as well as disorder effects caused by the Li-split positions are adressed,too. Various thermodynamic properties such as magnetization and magnetic specific heat are calculated and compare well with available experimental data. $LiSbCuO_4$ is found to be one of the most challenging edge-shared cuprates with unusual physical properties.

[1] S.E. Dutton *et al.*, PRL **108**, 187206 (2012).

TT 42.12 Wed 12:30 H18

Thermodynamic investigations of the quasi-2d triangular Heisenberg antiferromagnet $Cs_2CuCl_{4-x}Br_x$ ($x = 1, 2$) — •Ulrich Tutsch, Lars Postulka, Bernd Wolf, Michael Lang, Natalija van Well, Franz Ritter, Cornelius Krellner, and Wolf Assmus — Physikalisches Institut, Goethe-Universität Frankfurt (M), SFB/TR 49

$Cs_2CuCl_{4-x}Br_x$ ($0 \leq x \leq 4$) is a quasi-two-dimensional Heisenberg antiferromagnet with an anisotropic triangular in-plane coupling of the spins. The ratio J'/J of the spin-spin coupling constants determines the degree of frustration in the system and has been found to be 0.34 ($x = 0$) and 0.47 ($x = 4$) for the border compounds. In ref. [1] it has been suggested that for some intermediate Br concentration an even higher degree of frustration can be reached, and indeed, some results pointing into this direction have been reported by Ono *et al.* [2].

Here, we present specific heat C and susceptibility χ measurements below 1 K in magnetic fields B up to 13.5 T for the intermediate compounds $Cs_2CuCl_2Br_2$ and Cs_2CuCl_3Br, which, due to site-selective substitution [1], show a well-ordered halide sublattice. Our results, which point to a relatively high degree of frustration for $x = 2$, as well as the derived B-T phase diagram will be discussed in the framework of the triangular spin lattice.

[1] P.T. Cong *et al.*, Phys. Rev. B **83**, 064425 (2011)
[2] T. Ono *et al.*, J. Phys. Soc. Jpn. **74** Suppl., 135 (2005)

TT 42.13 Wed 12:45 H18

Spin relaxation processes in $Cr_{1-x}Fe_x$ — •S. Säubert[1,3], P. Schmakat[2,3], J. Kindervater[1], G. Benka[1], A. Bauer[1], J. N. Wagner[4], W. Häussler[3], O. Holderer[3], S. M. Shapiro[5], C. Pfleiderer[1], and P. Böni[2] — [1]Lehrstuhl für Topologie korrelierter Systeme, Technische Universität München, Garching, Germany — [2]Lehrstuhl für Neutronenstreuung, Technische Universität München, Garching, Germany — [3]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [4]Karlsruher Institute for Technology, IAM-WK, Eggenstein- Leopoldshafen, Germany — [5]Brookhaven National Laboratory, Department of Physics, Upton, USA

$Cr_{1-x}Fe_x$ shows reentrant spin glass behaviour below a doping dependent freezing temperature T_f. In contrast to a classical spin glass, the ground state changes from antiferromagnetic to ferromagnetic order with increasing iron concentration x [1, 2].

We report a study of the spin relaxation processes by means of neutron spin echo, magnetisation measurements and neutron depolarisation imaging for a wide range of concentrations x. This allows us to compare the relaxation process depending on the particular state at high temperatures. Our measurements provide an unprecedented combination of microscopic information on the spin dynamics and spin freezing on multiple length and time scales.

[1] S. K. Burke et al., J. Phys. F: Met. Phys. **13** 45 1-470 (1983)
[2] S. M. Shapiro et al., PRB **24**, 6661 (1981)
[3] R.M. Pickup et al., PRL **102**, 097202 (2009)

TT 43: Correlated Electrons: f-Electron & Heavy Fermion Systems

Time: Wednesday 9:30–13:00 Location: H20

TT 43.1 Wed 9:30 H20

Quantitative study of the f-occupation in $CeMIn_5$ and other cerium compounds with hard x-ray core level photo emission — •Martin Sundermann[1], Fabio Strigari[1], Thomas Willers[1], Jonas Weinen[2], Yen-Fa Liao[3], Ku-Ding Tsuei[3], Eric D. Bauer[4], John L. Sarrao[4], Joe D. Thompson[4], Pascal Lejay[5], Arata Tanaka[6], Liu Hao Tjeng[2], and Andrea Severing[1] — [1]University of Cologne, Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]National Syn-

chrotron Radiation Research Center, Hsinchu, Taiwan — [4]Los Alamos National Laboratory, Los Alamos, US — [5]Institut NEEL, CNRS, Grenoble, France — [6]Hiroshima University, Higashi-Hiroshima, Japan

Bulk-sensitive hard x-ray photoelectron spectroscopy (HAXPES) data of the Ce3*d* core levels of the CeMIn$_5$ family with M = Co, Rh, and Ir will be presented. The data analysis combines a full multiplet and configuration interaction model so that the strong plasmons intensities can be corrected for. This way spectral f^n weights can be extracted and the configuration interaction model yields quantitative values for the initial state f-occupation of the CeMIn$_5$. The results are compared with HAXPES data of other heavy Ce compounds of very different hybridization strength. A systematic decrease of the hybridization strength V_{eff} from $CePd_3$ to $CeRh_3B_2$ to $CeRu_2Si_2$ is observed, and it is smallest for the three CeMIn$_5$ compounds. The f-occupation increases in the same sequence and is close to one for the CeMIn$_5$ family.

TT 43.2 Wed 9:45 H20

Combined crystal field - phonon excitations in non-centrosymmetric heavy fermion $CeAuAl_3$ — •Petr Čermák[1], Astrid Schneidewind[1], Christian Franz[2,3], Rudolf Schönmann[2], Oleg Sobolev[3,4], and Christian Pfleiderer[2] — [1]Jülich Centre for Neutron Science, MLZ, Garching, DE — [2]Physik-Department, Technische Universität München, Garching, DE — [3]FRM II, Technische Universität München, Garching, DE — [4]Institute for Physical Chemistry, Georg-August-University, Göttingen, DE

Hybridized excitations that comprise of well-understood collective modes have received increasing interest as the possible origin of unconventional materials properties. In strongly correlated systems the effects of electron-phonon interactions are typically neglected, being deemed not important for the overall understanding. Recently, neutron experiment on $CeCuAl_3$ has provided putative evidence for a combined crystal field - phonon excitation [1]. In turn, an important question concerns to what extent these modes are a generic property, say, at least of the entire series of CeTAl$_3$ compounds (T: transition metal element) or even f-electron systems in a more general sense.

Our triple axis neutron measurement on single-crystal $CeAuAl_3$ revealed a new weakly dispersive excitation in contrast with earlier reports on polycrystals [2], suggesting rather generic phenomena. We have further proven, that this excitation is magnetically driven and is strongly connected with localized optical acoustic modes.

[1] D.T. Adroja et al., Phys. Rev. Lett. **108**, 216402 (2012)
[2] D.T. Adroja et al., Phys. Rev. B **91**, 134425 (2015)

TT 43.3 Wed 10:00 H20

Magnetic field dependence of spin fluctuations in CeB_6 — •P. Y. Portnichenko[1], A. V. Semeno[2], H. Ohta[3], A. S. Cameron[1], M. A. Surmach[1], H. Jang[4,5], G. Friemel[4], A. V. Dukhnenko[6], N. Yu. Shitsevalova[6], V. B. Filipov[6], A. Schneidewind[7], J. Ollivier[8], A. Podlesnyak[9], S. V. Demishev[2], and D. S. Inosov[1,4] — [1]TU Dresden, Germany — [2]GPI of RAS, Moscow, Russia — [3]Kobe University, Japan — [4]MPI Stuttgart, Germany — [5]SLAC, Stanford, USA — [6]IMPS, Kiev, Ukraine — [7]JCNS, Jülich, Germany — [8]ILL, Grenoble, France — [9]SNS, Oak Ridge, USA

The heavy fermion metal CeB_6 with a simple cubic crystal structure is characterized by a rich magnetic-field – temperature phase diagram. The zero-field antiferromagnetic ground state can be suppressed by an external field of only 1.7 T, above which an antiferroquadrupolar phase II is stabilized, resulting in a field-induced quantum critical point (QCP). Our recent inelastic neutron scattering (INS) studies have revealed a complex spectrum of low-energy collective excitations with intensity maxima at the Γ and R points. We have followed the magnetic field dependence of the excitation spectrum across the QCP. Our data reveal a nonmonotonic behavior of the strong ferromagnon mode at the Γ point, as it initially gets suppressed and becomes quasielastic, but then develops into a collective mode within phase II. At high fields, it follows the same linear behavior as one of the recently discovered electron-spin resonances, proving the common origin of these excitations. An even more complex field dependence was also observed at the R point, where a second low-energy mode emerges in phase II.

TT 43.4 Wed 10:15 H20

Quantum Oscillations without a Fermi Surface – the Anomalous de Haas-van Alphen Effect and relation to SmB_6 — •Johannes Knolle and Nigel Cooper — T.C.M. Group, Cavendish Laboratory, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

The de Haas-van Alphen effect (dHvAE), describing oscillations of the magnetization as a function of magnetic field, is commonly assumed to be a definite sign for the presence of a Fermi surface (FS). Indeed, the effect forms the basis of a well-established experimental procedure for accurately measuring FS topology and geometry of metallic systems, with parameters commonly extracted by fitting to the Lifshitz-Kosevich (LK) theory based on Fermi liquid theory. Here we show that, in contrast to this canonical situation, there can be quantum oscillations even for band insulators of certain types. We provide simple analytic formulas describing the temperature dependence of the quantum oscillations in this setting, showing strong deviations from LK theory. We draw connections to recent experiments on the tentative topological Kondo insulator SmB_6.

TT 43.5 Wed 10:30 H20

Valence fluctuations in the boride $Eu_4Pd_{29+x}B_8$ — •Roman Gumeniuk[1], Walter Schnelle[2], Mahmoud Ahmida[3], Mohsen Abd-Elmeguid[3], Kristina Kvashnina[4], Alexander Tsirlin[2], Andreas Leithe-Jasper[2], and Christoph Geibel[2] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Straße 23, 09596 Freiberg, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden, Germany — [3]Universität zu Köln, II. Physikalisches Institut, Zülpicher Str. 77, 50937 Köln, Germany — [4]ESRF, 71, Avenue des Martyrs, Grenoble France

We synthesized a high quality sample of the boride $Eu_4Pd_{29+x}B_8$ (x = 0.76) and studied its structural and physical properties. Its tetragonal structure was solved by direct methods and confirmed to belong to the $Eu_4Pd_{29}B_8$ type. All studied physical properties indicate a valence fluctuating Eu state, with a valence decreasing continuously from about 2.9 at 5 K to 2.7 at 300 K. Maxima in the T dependence of the susceptibility and thermopower at around 135 K and 120 K, respectively, indicate a valence fluctuation energy scale on the order of 300 K. Analysis of the susceptibility evidences some inconsistencies when using the ionic interconfigurational fluctuation (ICF) model, thus suggesting a stronger relevance of hybridization between $4f$ and valence electrons compared to standard valence-fluctuating Eu systems.

TT 43.6 Wed 10:45 H20

Coexistence of magnetic order and valence fluctuations in a heavy fermion system $Ce_2Rh_3Sn_5$. — •Monika Gamza[1,2,4], Roman Gumeniuk[3,2], Walter Schnelle[2], Ulrich Burkhardt[2], Andrzej Ślebarski[4], and Helge Rosner[2] — [1]Jeremiah Horrocks Institute, University of Central Lancashire, Preston, UK — [2]MPI CPfS, Dresden, Germany — [3]Institute of Experimental Physics, Freiberg University of Mining and Technology, Freiberg, Germany — [4]Institute of Physics, University of Silesia, Katowice, Poland

While most Ce-based intermetallics contain either trivalent or intermediate-valent Ce ions, only for a few compounds a coexistence of both species has been reported. Here, we present a combined experimental and theoretical study based on thermodynamic measurements and spectroscopic data together with ab-initio electronic structure calculations aiming at exploring magnetic properties of Ce ions in two nonequivalent sites in $Ce_2Rh_3Sn_5$. Ce L_{III} XAS spectra give direct evidence for valence fluctuations. Magnetization measurements show an onset of an antiferromagnetic order at $T_N \approx 2.5$ K. The electronic structure calculations suggest that the magnetic ordering is related only to one Ce sublattice. This is in-line with a small entropy associated with the magnetic transition $S_{\text{mag}} \approx 0.35$ R ln2 per Ce atom as revealed by the specific heat measurement. Furthermore, the temperature dependence of the magnetic susceptibility can be well described assuming that there are fluctuating moments of Ce^{3+} ions in one sublattice, whereas Ce atoms from the second sublattice are in a nonmagnetic intermediate valence state.

TT 43.7 Wed 11:00 H20

Exchange field effect in the crystal field ground state of CeMAl$_4$Si$_2$ — •Kai Chen[1], Fabio Strigari[1], Martin Sundermann[1], Stefano Agrestini[2], Eric D. Bauer[3], John L. Sarrao[3], Joe D. Thompson[3], Edwige Otero[4], Arata Tanaka[5], and Andrea Severing[1] — [1]University of Cologne, Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]Los Alamos National Laboratory, Los Alamos, US — [4]Synchrotron Soleil,Gif-sur-Yvette Cedex,France — [5]Hiroshima University, Higashi-Hiroshima,Japan

The crystal-field ground state wave functions of the tetragonal Kondo lattice materials CeMAl$_4$Si$_2$(M = Rh, Ir and Pt), as well as the

crystal-field splittings, are determined with low temperature linear polarized soft x-ray absorption spectroscopy. Surprisingly, at T < 20 K, which is far below the first excited crystal-field level at 200 K, a change in linear dichroism was observed that cannot be accounted for by population of crystal-field states. Adding an exchange field to the ionic full multiplet calculations below 20 K leads to a splitting to the ground state doublet and modification of J_z admixture, thus accounting for the change in low temperature linear dichroism. The direction of the required exchange field is parallel along c-axis for the antiferromagnetic Rh and Ir compounds, and perpendicular to c-axis for ferromagnetic $CePtAl_4Si_2$.

15 min. break

TT 43.8 Wed 11:30 H20

Single crystal growth and low-temperature properties of Er_3Al_2 — •Christian Suttner, Georg Benka, Andreas Bauer, and Christian Pfleiderer — Physik Department, Technische Universität München, D-85748 Garching, Germany

In recent years, topologically non-trivial spin whirls in condensed matter systems attracted great scientific interest. Lattices of these objects, so-called magnetic skyrmion lattices, were mainly observed in Dzyaloshinskii-Moriya driven chiral magnets with the non-centrosymmetric cubic space group $P2_13$ [1,2]. Similar spin textures, however, may in principle also arise in a large number of further compounds. We report single-crystal growth of Er_3Al_2 crystallizing in the tetragonal space group $P4_2/mnm$ by means of optical float zoning under UHV-compatible conditions. We determined the magnetic phase diagram for fields applied along different crystallographic directions using magnetization, ac susceptibility, and specific heat measurements. Several phase pockets are observed below the Néel temperature $T_N = 27\,K$, consistent with earlier reports [3].

[1] S. Mühlbauer *et al.*, Science **323**, 915 (2009)
[2] N. Nagaosa and Y. Tokura, Nature Nanotech. **8**, 899 (2013)
[3] R. L. Davis *et al.*, Mater. Sci. Forum **27–28**, 249 (1988).

TT 43.9 Wed 11:45 H20

Synthesis and Characterisation of YbPdSb — •Charles R. S. Haines, Philip A. C. Brown, and Friedrich M. Grosche — Department of Physics, Cavendish Laboratory, University of Cambridge, UK

The intermetallic compound YbPdSb can form in two structures: the low temperature (LT) half-Heusler phase, in which the Yb atoms form a frustrated fcc structure, and the high temperature (HT) Pnma modification. We have prepared phase pure samples of both structures and report resistivity, magnetisation and heat capacity measurements on both. The LT phase is a Kondo lattice system [1] showing large-moment Curie-Weiss paramagnet behaviour without any phase transition anomalies down to the lowest temperatures measured. The resistivity is rather insensitive to temperature from room temperature down to ∼50K where it decreases steeply with further cooling. By contrast, in the HT phase the magnetic susceptibility displays weak temperature dependence and the resistivity falls with decreasing temperature in the way expected of a weakly correlated metal. These findings suggest that in contrast to the electronic state in the LT structure, the 4f-shell of Yb is completely filled in the HT structure of YbPdSb, presenting an interesting opportunity to study the interplay between lattice and electronic structure within the same compound.

[1] H. Suzuki et al., Physica B: Condensed Matter **206-207**, 341 (1995).

TT 43.10 Wed 12:00 H20

Variational cluster approach to superconductivity in the Kondo lattice model — •Benjamin Lenz, Salvatore R. Manmana, and Thomas Pruschke — Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany

The variational cluster approximation (VCA) allows to study broken symmetry phases of various lattice models at zero temperature. However, most research has been done on electron systems without coupling to additional spins. Here, we investigate the Kondo lattice model (KLM) - a paradigmatic model for heavy fermion materials which contains interactions between electrons and localized spins. We first focus on the antiferromagnetic ground state in the half-filled KLM and compare our finite-size extrapolated VCA results to those of other established techniques, like quantum Monte Carlo. We further ask for the existence of superconductivity at finite doping in this model, motivated by findings for heavy fermion systems and dynamical mean-field theory (DMFT)[1]. We probe the system for s- and d-wave superconductivity and present an analysis of the different ground states which emerge on tuning the electron filling and exchange coupling strength J.

Financial support via DFG through FOR1807 is gratefully acknowledged.

[1] O. Bodensiek, R. Zitko, M. Vojta, M. Jarrell, and T. Pruschke, PRL **110**, 146406 (2013)

Invited Talk TT 43.11 Wed 12:15 H20

Rare-earth-like behavior of transition metals substituted in Li_3N — •Anton Jesche — EP 6, Electronic Correlations and Magnetism, University of Augsburg, Germany

Large magnetic anisotropy and coercivity are key properties of functional magnetic materials and are generally associated with rare-earth elements. The magnetic anisotropy of 3d transition metals, on the other hand, is usually considered to be weak. Main reason is the widely known paradigm of orbital quenching. However, a rare interplay of crystal electric field effects and spin-orbit coupling causes a large orbital contribution to the magnetic moment of the $T = \{$Mn, Fe, Co and Ni$\}$ in $Li_2(Li_{1-x}T_x)N$. Accordingly, extremely large magnetic anisotropies have been found. Most notably, the magnetic anisotropy alternates as easy plane → easy axis → easy plane → easy axis when progressing from T = Mn → Fe → Co → Ni [1].

Furthermore, experimental evidence for a macroscopic quantum tunneling of the magnetization has been observed in diluted $Li_2(Li_{1-x}Fe_x)N$ with $x \ll 1$. Steps in the hysteresis loops and relaxation phenomena in striking similarity to single-molecule magnets indicate the presence of nanoscale magnetic centers, which are likely built from single, isolated iron atoms [2]. Recent results are going to be discussed and contrasted with established molecular magnets, hard permanent magnets and rare-earth-based model systems.

[1] A. Jesche *et al.* Phys. Rev. B **91**, 180403(R) (2015)
[2] A. Jesche *et al.*, Nature Comm. **5**:3333
doi: 10.1038/ncomms4333 (2014)

TT 43.12 Wed 12:45 H20

Thin Film Fabrication and Transport Properties of the Heavy Fermion Oxide LiV_2O_4 — •Ulrike Niemann[1], Daigorou Hirai[2], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Tokyo, Tokyo, Japan — [3]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Stuttgart, Germany

The spinel compound LiV_2O_4 is well-known for its heavy fermion behaviour, although it contains no f-electron bands [1],[2]. This unexpected behaviour has been a subject of several studies, but the origin of it is still not fully understood. In this study, we successfully fabricated single crystalline epitaxial thin film of LiV_2O_4 on $SrTiO_3$, LSAT and MgO substrates, using a pulsed laser deposition technique. By changing film thickness and substrate materials, dimensionality and epitaxial strain was controlled. The formation of an epitaxially grown LiV_2O_4 phase has been confirmed by X-ray diffraction measurements. LiV_2O_4 films on MgO were found to be strained, due to the small lattice mismatch, in contrast to fully relaxed films on $SrTiO_3$.The heavy fermion behaviour of bulk LiV_2O_4 at low temperatures is well reproduced in thick enough (≈ 7 nm) films on $SrTiO_3$ substrates. In contrast, an insulating phase was found in strained LiV_2O_4 thin films on MgO substrates, revealing the key role of the lattice in stabilising the metallic ground state. In this presentation, we discuss the thin film fabrication and the effect of epitaxial strain on heavy fermion behaviour in LiV_2O_4.

[1] S. Kondo et al., PRL **78**, 3729 (1997)
[2] C. Urano et al., PRL **85**, 1052 (2000)

TT 44: Transport: Graphene (Joint session of DS, DY, HL, MA, O and TT organized by TT)

Time: Wednesday 9:30–13:15 Location: H22

Invited Talk TT 44.1 Wed 9:30 H22

Ultrafast photo-thermoelectric currents in graphene — •Alexander Holleitner — Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, D-85748 Garching, Germany.

We show that photo-thermoelectric currents occur on a picosecond time-scale in graphene [1]. To this end, we apply an on-chip pump/probe photocurrent spectroscopy [2,3] to double-gated junctions of graphene. Our experiments reveal the interplay of photogenerated hot electrons with so-called photovoltaic currents. Moreover, we demonstrate that hot electrons allow to read-out an ultrafast non-radiative energy transfer from fluorescent emitters, namely nitrogen-vacancy centers in nano-diamonds. The non-radiative energy transfer can be exploited as an ultrafast, electronic read-out process of the electron spin in nitrogen vacancy centers in the diamond nanocrystals. The detection gives access to fast energy transfer processes, which have not yet been observed by fluorescence measurements because of quenching of the optical signal for short transfer distances [4].

We thank A. Brenneis, F. Schade, L. Gaudreau, M. Seifert, H. Karl, M.S. Brandt, H. Huebl, J.A. Garrido, F.H.L. Koppens, for a very fruitful collaboration, and the ERC-grant 'NanoREAL' for financial support.

[1] A. Brenneis et al., (2016)
[2] L. Prechtel et al., Nature Comm. **3**, 646 (2012)
[3] C. Kastl et al. Nature Comm. **6**, 6617 (2015)
[4] A. Brenneis et al. Nature Nanotech. **10**, 135 (2015)

TT 44.2 Wed 10:00 H22

Double-logarithmic velocity renormalization at the Dirac points of graphene — •Peter Kopietz, Anand Sharma, and Carsten Bauer — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Str. 1, 60438 Frankfurt

Using a functional renormalization group approach with partial bosonization in the forward scattering channel we reconsider the effect of long-range Coulomb interactions on the quasi-particle velocity v_k close to the Dirac points of graphene. In contrast to calculations based on perturbation theory and field theoretical renormalization group methods, we find that v_k is proportional to $\ln[\kappa_k/k]$ where k is the deviation of the quasiparticle momentum from the Dirac points and the cutoff scale κ_k vanishes logarithmically for small k. We show that this double-logarithmic singularity is compatible with experiments and with the known three-loop expansion of v_k which contains terms of order $\ln k$ and $\ln^2 k$.

TT 44.3 Wed 10:15 H22

Dirac fermion wave packets in oscillating potential barriers — Walter Pötz[1], Sergey E. Savel'ev[2], Peter Hänggi[3], and •Wolfgang Häusler[3] — [1]Karl Franzens Univ. Graz, Inst. Phys., A-8010 Graz, Austria — [2]Department of Physics, Loughborough University, Loughborough LE11 3TU, United Kingdom — [3]Institut für Physik, Univ. Augsburg, 86135 Augsburg, Germany

We integrate the time-dependent (2+1)D Dirac equation for massless fermions in graphene or topological insulator surfaces. A recently developed staggered-grid leap-frog scheme is employed [1,2]. We consider an initial Gaussian wave packet which moves in the x-direction towards a potential barrier that is homogeneous along y and oscillates periodically in time. As for the x-dependence, we investigate square-well, sinusoidal, and linear-ramp potential profiles. Small transversal momentum components k_y of the wave packet were analyzed analytically [3] and predicted to generate non-zero current densities j_y, even at normal incidence $k_y = 0$ [4]. These findings are consistent with the present numerical studies of particle-, current-, and spin-density. We also investigate massive fermions: regarding some properties they resemble massless fermions, regarding other properties, however, peculiar intrinsic oscillations, reminiscent of Zitterbewegung, appear.

[1] R. Hammer and W. Pötz, PRB **88**, 235119 (2013)
[2] R. Hammer *et al.*, J. Comp. Phys. **265**, 50 – 70 (2014)
[3] S.E. Savel'ev, W. Häusler, and P. Hänggi, PRL **109**, 226602 (2012)
[4] S.E. Savel'ev, W. Häusler, and P. Hänggi, EPJB **86**, 433 (2013).

TT 44.4 Wed 10:30 H22

Electric and magnetic control of electron guiding in graphene — •Ming-Hao Liu and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg

Electrons in graphene are known to behave like massless Dirac fermions, whose transport properties can be best revealed by experiments using ultra-clean graphene. Reliable quantum transport simulations for ballistic graphene is naturally a powerful tool for understanding and predicting high-quality transport experiments. In this talk we show gate-controlled electron guiding along electrically confined channels in suspended graphene, which is a combined work of our transport simulations and the experiment done by the Schönenberger group [1]. We have recently further applied our simulation (Green's function method within the scalable tight-binding model [2]) to revisit the transverse magnetic focusing experiment [3], where the guiding of the electrons is controlled by an external magnetic field, instead of electrical gates. Besides good agreement with the experiments [1,3], our simulations further allow for probing charge flow through an additional scanning probe tip.

[1] P. Rickhaus *et al.*, Nano Lett. **15**, 5819 (2015).
[2] M.-H. Liu *et al.*, Phys. Rev. Lett. **114**, 036601 (2015).
[3] T. Taychatanapat *et al.*, Nat. Phys. **9**, 225 (2013).

TT 44.5 Wed 10:45 H22

Current flow paths in deformed graphene: from quantum transport to classical trajectories in curved space — •Nikodem Szpak[1] and Thomas Stegmann[1,2] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [2]Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca

We compare two contrasting approaches to the electronic transport in deformed graphene: a) the condensed matter approach in which current flow paths are obtained by applying the non-equilibrium Green's function (NEGF) method to the tight-binding model with local strain, b) the general relativistic approach in which classical trajectories of relativistic point particles moving in a curved surface with a pseudo-magnetic field are calculated. The connection between the two is established in the long-wave limit via an effective Dirac Hamiltonian in curved space. Geometrical optics approximation, applied to focused current beams, allows us to directly compare the wave and the particle pictures. We obtain very good numerical agreement between the quantum and the classical approaches for a fairly wide set of parameters. The presented method offers an enormous reduction of complexity from irregular tight-binding Hamiltonians defined on large lattices to geometric language for curved continuous surfaces. It facilitates a comfortable and efficient tool for predicting electronic transport properties in graphene nanostructures with complicated geometries, paving the way to new interesting transport phenomena such as bending or focusing (lensing) of currents depending on the shape of the deformation. It can be applied in designing ultrasensitive sensors or in nanoelectronics.

TT 44.6 Wed 11:00 H22

Trigonal Warping in Bilayer Graphene: Energy versus Entanglement Spectrum — •Sonja Predin, Paul Wenk, and John Schliemann — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We present a mainly analytical study of the entanglement spectrum of Bernal-stacked graphene bilayers in the presence of trigonal warping in the energy spectrum. Upon tracing out one layer, the entanglement spectrum shows qualitative geometric differences to the energy spectrum of a graphene monolayer. However, topological quantities such as Berry phase type contributions to Chern numbers agree. The latter analysis involves not only the eigenvalues of the entanglement Hamiltonian but also its eigenvectors. We also discuss the entanglement spectra resulting from tracing out other sublattices.

15 min. break

TT 44.7 Wed 11:30 H22

Valley-based Cooper pair splitting via topologically confined channels in bilayer graphene — •Alexander Schroer[1], Peter G. Silvestrov[1], and Patrik Recher[1,2] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106

Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology Braunschweig, D-38106 Braunschweig, Germany

Bilayer graphene hosts valley-chiral one-dimensional modes at domain walls between regions of different interlayer potential or stacking order. When such a channel is close to a superconductor, the two electrons of a Cooper pair, which tunnel into it, move in opposite directions because they belong to different valleys related by the time-reversal symmetry. This kinetic variant of Cooper pair splitting requires neither Coulomb repulsion nor energy filtering but is enforced by the robustness of the valley isospin in the absence of atomic-scale defects. We derive an effective normal/superconducting/normal (NSN) model of the channel in proximity to an *s*-wave superconductor, calculate the conductance of split and spin-entangled pairs, and interpret it as a result of *local* Andreev reflection, in contrast to the widespread identification of Cooper pair splitting with crossed Andreev reflection in an NSN geometry.

TT 44.8 Wed 11:45 H22

The decisive role of stacking faults for understanding transport in bilayer graphene — •Heiko B. Weber[1], Ferdinand Kisslinger[1], Christian Ott[1], and Sam Shallcross[2] — [1]Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg (FAU), Erlangen, Germany — [2]Lehrstuhl für Theoretische Festkörperphysik, FAU Erlangen-Nürnberg (FAU)

Charge transport in bilayer graphene provides rich low-temperature phenomena, often assigned to interaction-driven phase transitions. We will discuss charge transport in bilayer graphene in a single-particle picture, but including stacking faults. Such partial dislocations are unavoidable in bilayer graphene and were recently imaged [1]. Depending on details, partial dislocations can introduce improved conductance, fully insulating behaviour or linear magnetoresistance. The latter is reliably found in transport experiments at elevated temperatures [2].

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer, E. Spiecker, Nature **505**, 533 (2014)
[2] F. Kisslinger, C. Ott, C. Heide, E. Kampert, B. Butz, E. Spiecker, S. Shallcross, H. B. Weber, Nature Phys. **11**, 650 (2015).

TT 44.9 Wed 12:00 H22

Linear magnetoresistance in two-dimensional disordered conductors — •Ferdinand Kisslinger[1], Christian Ott[1], Erik Kampert[2], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg (FAU), Erlangen, Germany. — [2]Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany.

The recent observation of linear magnetoresistance (MR) in large-area bilayer graphene gives a key to the understanding of this old and barely understood phenomenon [1]. In bilayer graphene, it can be traced back to mosaic-like pattern of a partial dislocation network [2]. In this talk we discuss how linear MR evolves in disordered samples, using a two dimensional resistor network model conceptually introduced by Parish and Littlewood [3]. This model is in the weak disorder regime dominated by boundary effects. We identified a new regime representing the bulk situation in a disordered conductor. We investigated different possible sources of disorder: mobility, charge carrier density and network structure. The slope of the MR turned out to be simply governed by the Hall resistance and therefore by the inverse of the charge carrier density. An equivalent circuit model finally gives a consistent explanation as to why the magnetoresistance is linear in mosaic like samples.

[1] F. Kisslinger et al., Nature Physics **11**, 650 (2015)
[2] B. Butz et al., Nature **505**, 533 (2014).
[3] M. M. Parish & P. B. Littlewood, Nature **426**, 162 (2003)

TT 44.10 Wed 12:15 H22

Mechanically strained graphene nanojunctions — •Seddigheh Nikipar[1], Dmitry Ryndyk[1], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Germany

It has been demonstrated recently that mechanically strained graphene presents interesting electrical properties, which have great potential for novel applications in electronic devices. In particular, the strain in graphene nanoribbons can lead to substantial changes in its electronic properties. Besides, it provides a possibility to develop atomic point contacts and break junctions. The main purpose of this work is to investigate theoretically the influence of uniaxial mechanical strains on graphene nanojunctions in order to design graphene point contact.

To this aim, we developed the computational model by combining density functional theory and molecular dynamics methods. First, we investigated the change of the junction shape with increasing strain and the breaking with the formation of the nanogap. As expected, our theoretical model predicts the deformation of the break junction bottleneck into carbon chains before the rupture of the structure. we evaluated the electronic transmission function of graphene quantum junction by employing a coupled tight bonding and nonequilibrium green function methods. Interestingly it is found that graphene point contact can present resonance transmission in contrast to the conventional metallic point contacts with quantized conductance. This might be originated from influence of other parameters on transmission.

TT 44.11 Wed 12:30 H22

Graphene nanoribbons as effective spin ladders — •Cornelie Koop, Manuel J. Schmidt, and Stefan Wessel — Institut für Theoretische Festkörperphysik, RWTH Aachen University

Zigzag edges of graphene nanoribbons host particular, localized edge states. Since the density of states is strongly enhanced near the edges in graphene, interaction effects between the spins of these edge states become important. We can significantly simplify the analysis of such systems by means of an effective model that separates the edge and bulk states. Treating the effective interactions to first order proves sufficient in most cases, while second order corrections do not dramatically change the results. In many cases, the edge system can be reduced to a general spin ladder model, where the decay of the spin-spin interaction is determined by the shape of the edges. We examine these effective spin ladders at finite temperatures by means of quantum Monte Carlo simulations, using the stochastic series expansion method. Thereby, correlation functions and spin structure factors can be determined for realistically large graphene nanoribbons.

TT 44.12 Wed 12:45 H22

Edge State Structure of the $\nu = 0$ quantum Hall State in monolayer Graphene — •Angelika Knothe[1,2] and Thierry Jolicoeur[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — [2]Université Paris 11, CNRS, LPTMS, UMR 8626, Orsay 91405 France

Single-layer graphene at neutrality under a magnetic field is a many-body insulator whose phase structure is under intense scrutiny. When tilting the applied magnetic field, there is a phase transition towards a conducting state [1]. A plausible description is to start from a SU(4) spin-valley symmetric quantum Hall ferromagnet and add some lattice-scale anisotropies in valley space [2]. In the manifold of ground states captured by this approach, it has been proposed that graphene undergoes a transition between a canted antiferromagnetic state and a ferromagnetic state. While this picture is clear in the bulk of the system, it remains to understand the effect of this phase change on the current-carrying edge states that are formed a the physical boundaries of a real sample [3]. We use an extended Hartree-Fock approach to describe a finite-size system with a simple model for the edge and extract the one-body spectrum. We then describe the current-carrying edge textures.

[1] A. F. Young et al., Nature (London) 505, 528 (2014) [2] M. Kharitonov, Phys. Rev. B 85, 155439 (2012) [3] M. Kharitonov, Phys. Rev. B 86, 075450 (2012); G. Murthy et al., Phys. Rev. B 90, 241410 (2014) and arXiv:1510.04255; A. Knothe and T. Jolicoeur, Phys. Rev. B 92, 165110 (2015)

TT 44.13 Wed 13:00 H22

Spin lifetimes exceeding 12 ns in graphene non-local spin valves at room temperature — •Christopher Franzen[1], Marc Drögeler[1], Frank Volmer[1], Tobias Pohlmann[1], Maik Wolter[1], Kenji Watanabe[2], Takashi Taniguchi[2], Christoph Stampfer[1], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

We present spin transport measurements on graphene non-local spin transport devices by fabricating the electrodes first and subsequently transfer graphene with hexagonal boron nitride on top [1]. We achieve spin lifetimes of 12.6 ns and a spin diffusion length as high as 30 μm at room temperature.

This improvement exceeds all current models for contact-induced spin dephasing which paves the way towards probing intrinsic spin properties of graphene. Furthermore, we investigate the contact properties

of our devices using scanning force microscopy (SFM) and conductive SFM. We discuss the importance of using large area hexagonal boron nitride for the transfer process and for achieving such high spin lifetimes and spin diffusion lengths.

[1] M. Drögeler *et al.* Nano Letters **14**, 6050 (2014).

TT 45: Spintronics (incl. Quantum Dynamics) (Joint session of MA, HL and TT organized by MA)

Time: Wednesday 9:30–12:15 Location: H32

TT 45.1 Wed 9:30 H32

Valley polarization in magnetically doped single-layer transition-metal dichalcogenides — •Udo Schwingenschlögl, Yingchun Cheng, and Qingyun Zhang — PSE Division, KAUST, Thuwal 23955, Saudi Arabia

We demonstrate that valley polarization can be induced and controlled in semiconducting single-layer transition-metal dichalcogenides by magnetic doping, which is important for spintronics, valleytronics, and photonics devices. As an example, we investigate Mn-doped MoS_2 by first-principles calculations. We study how the valley polarization depends on the strength of the spin orbit coupling and the exchange interaction and discuss how it can be controlled by magnetic doping. Valley polarization by magnetic doping is also expected for other honeycomb materials with strong spin orbit coupling and the absence of inversion symmetry. Reference: Phys. Rev. B **89**, 155429 (2014).

TT 45.2 Wed 9:45 H32

Giant Rashba-type spin splitting in ferroelectric GeTe(111) — •Marcus Liebmann[1], Christian Rinaldi[2], Domenico Di Sante[3], Jens Kellner[1], Christian Pauly[1], Rui Ning Wang[4], Jos Emiel Boschker[4], Alessandro Guissani[4], Stefano Bertoli[2], Matteo Cantoni[2], Lorenzo Baldrati[2], Marco Asa[2], Ivana Vobornik[5], Giancarlo Panaccione[5], Dmitry Marchenko[6], Jaime Sanchez-Barriga[7], Oliver Rader[7], Raffaella Calarco[4], Silvia Picozzi[3], Riccardo Bertacco[2], and Markus Morgenstern[1] — [1]II. Inst. Phys. B, RWTH Aachen University — [2]Politecnico di Milano, Italy — [3]Consiglio Nazionale delle Ricerche, L'Aquila, Italy — [4]Paul-Drude-Institut für Festkörperelektronik, Berlin — [5]Consiglio Nazionale delle Ricerche, Trieste, Italy — [6]Physikalische und Theoretische Chemie, Freie Universität Berlin — [7]Helmholtz-Zentrum für Materialien und Energie, BESSY, Berlin

The ferroelectric semiconductor GeTe has been proposed to exhibit a giant spin splitting of bulk Rashba bands with spin rotation direction coupled to the dielectric polarization [1]. We probe GeTe(111) grown by MBE using in-situ angular-resolved photoelectron spectroscopy (ARPES). We identify a novel Rashba-split surface band with giant spin splitting and find signatures of the bulk Rashba band by comparison with density functional theory calculations [2]. The ferroelectric polarization, as determined by piezo force microscopy, agrees with the predicted helical spin-momentum relation of the Rashba bands.

[1] D. Di Sante *et al.*, Adv. Mater. **25**, 509 (2013).

[2] M. Liebmann *et al.*, Adv. Mater. 2015, 10.1002/adma.201503459.

TT 45.3 Wed 10:00 H32

Spin Mapping of Surface and Bulk Rashba States in Ferroelectric α-GeTe(111) Films — •H. J. Elmers[1], R. Wallauer[1], M. Liebmann[2], J. Kellner[2], M. Morgenstern[2], R.N. Wang[3], J.E. Boschker[3], R. Calarco[3], O. Rader[4], D. Kutnyakhov[1], S.V. Chernov[1], K. Medjanik[1], C. Tusche[5], M. Ellguth[5], H. Volfova[6], J. Braun[6], J. Minar[6], H. Ebert[6], and G. Schönhense[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz — [2]II. Physikalisches Institut B and JARA-FIT, RWTH Aachen — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — [5]Max Planck Institute for Microstructure Physics, Halle — [6]Department Chemie, Ludwig-Maximilians-Universität München

Ferroelectric semiconductors like GeTe promise a switchable Rashba-parameter for electronic bulk states. A comprehensive mapping of the spin polarization of the electronic bands in α-GeTe(111) films has been performed using a time-of-flight momentum microscope equipped with an imaging spin filter that enables a simultaneous measurement of more than 10.000 data points. In addition to the Rashba type splitting of surface bands we observe a spin splitting of bulk bands with opposite spin helicity of the inner and outer Rashba bands revealing the complex spin texture at the Fermi energy that determines electronic transport.

TT 45.4 Wed 10:15 H32

Optically and thermally driven spin dynamics and quantum Otto cycles on Ni_4 structures — •Stefan Sold[1], Bhaskar Kamble[2], Georgios Lefkidis[1], and Wolfgang Hübner[1] — [1]Departement of physics, University of Kaiserslautern and Research Center OPTIMAS, Germany — [2]Asia Pacific Center for Theoretical Physics, Pohang, Korea

We present two different kinds of combined optical and thermodynamic processes on the chain-like prototypical Ni_4 cluster, described on the basis of high-level quantum chemistry. The one consists of incoherent spin relaxation and thermalization processes, the other one of a nano Otto engine.

First, we model various temperature profiles by coupling to one or two temperature baths. The system dynamics is mathematically described with the Lindblad superoperator [1]. We find that the inhomogeneous temperature profile, giving rise to non-equilibrium mixed states, induces non-uniform spin-density distribution (spin Seebeck effect on the nano scale).

Second, we propose a quantum Otto motor [2], which benefits from the spin degree of freedom and the energy discretization of the cluster, and may thus surpass the efficiency limit of classical Carnot cycles [3].

[1] G. Schaller and T. Brandes, Phys. Rev. A **78**, 022106 (2008)

[2] W. Hübner, G. Lefkidis, C. D. Dong, D. Chaudhuri, L. Chotorlishvili, and J. Berakdar, Phys. Rev. B **90**, 024401 (2014)

[3] C. D. Dong, G. Lefkidis, and W. Hübner, Phys. Rev. B **88**, 214421 (2013)

TT 45.5 Wed 10:30 H32

Theoretical aspects of the Edelstein effect for anisotropic 2DEGs and topological insulators — •Annika Johansson[1,2], Dmitry Fedorov[1,2], Jürgen Henk[2], and Ingrid Mertig[2,1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

A charge current driven through a two-dimensional electron gas (2DEG) with Rashba spin-orbit coupling [1] generates a spatially homogeneous spin polarization perpendicular to the applied electric field. This phenomenon is the Edelstein effect [2].

For selected model systems, we consider the Edelstein effect within the semiclassical Boltzmann transport theory. Its energy dependence is investigated, in particular the regime below the Dirac point of the 2DEG. In addition to an isotropic 2DEG [1], we analyze systems with anisotropic Fermi contours. We predict that the current-induced spin polarization vanishes if the Fermi contour passes through a Lifshitz transition. In addition, we corroborate that topological insulators provide a very efficient conversion of charge to spin current [3].

Our findings for paradigmatic Rashba systems call for experimental verification.

[1] Y. Bychokov and E. Rashba, J. Phys. C, **17**, 6039 (1984) [2] V. M. Edelstein, Solid State Commun., **73**, 233 (1990) [3] J. C. Rojas Sánchez *et al.*, ArXiv: 1509.02973 (2015)

15 min. break

TT 45.6 Wed 11:00 H32

Spin superfluidity and long-range transport in thin-film ferromagnets — Hans Skarsvåg, •Cecilia Holmqvist, and Arne Brataas — Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

In ferromagnets, magnons may condense into a single quantum state. Analogous to superconductors, this quantum state may support transport without dissipation. Recent works suggest that longitudinal spin transport through a thin-film ferromagnet is an example of spin su-

perfluidity. Although intriguing, this tantalizing picture ignores long-range dipole interactions; here, we demonstrate that such interactions dramatically affect spin transport. In single-film ferromagnets, "spin superfluidity" only exists at length scales (a few hundred nanometers in yttrium iron garnet) somewhat larger than the exchange length. Over longer distances, dipolar interactions destroy spin superfluidity. Nevertheless, we predict the re-emergence of spin superfluidity in tri-layer ferromagnet-normal metal-ferromagnet films that are ~1 micrometre in size. Such systems also exhibit other types of long-range spin transport in samples that are several micrometers in size.

TT 45.7 Wed 11:15 H32

Ultra-long electron and hole spin lifetimes in monolayer WSe_2 — Sammy Pissinger, •Robin de Winter, Christopher Franzen, Manfred Ersfeld, Sebastian Kuhlen, Christoph Stampfer, and Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, Germany

There is strong interest in optical generation and detection of valley spin polarizations in transition metal dichalcogenides. We report on time-resolved two color pump probe Kerr rotation measurements on mechanically exfoliated monolayer WSe_2 crystals. We find electron and hole spin lifetimes of up to 100 ns at low temperatures. These values are in good agreement with exciton lifetimes extracted from all-optical time-resolved reflectivity indicating that the spin lifetimes are limited by exciton recombination times in our crystals. Electron spin precession in Voigt geometry furthermore reveals inhomogeneous spin dephasing caused by a large spread in the local g factors.

TT 45.8 Wed 11:30 H32

Bulk Spin-Orbit Torques at finite temperatures in Bulk Half-Metallic Heuslers from First Principle — •Jacob Gayles[1], Libor Šmejkal[2], Jakub Železny[2], Frank Freimuth[3], Zhe Yuan[1], Yuriy Mokrousov[3], Tomas Jungwirth[2], and Jairo Sinova[1] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany — [2]Institute of Physics ASCR, v.v.i., Cukrovarnicka 10, 162 53 Praha 6 Czech Republic — [3]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We predict bulk spin-orbit torques in the half-metallic Heuslers NiMnSb and PtMnSb, using symmetry arguments in conjunction with first principle calculations. We present under uniaxial growth strain a linear dependence of the even torque and that can be tuned to zero while observing a sizable odd torque is independent of strain. Furthermore, these effects are seen to be two orders of magnitude larger in the PtMnSb. The even torque is strongly dependent on the temperature decreasing by 75% at room temperature where finite temperature is taken into account in the frozen phonon approximation. We show the equivalence of two widely used methods, the Landauer-Bütikker and the Kubo linear response formalism giving confidence in our result for experimental measurements in bulk magnetic Heusler compounds breaking inversion symmetry.

TT 45.9 Wed 11:45 H32

Dynamics of bound monopoles in artificial spin ice: How to store energy in Dirac strings. — •Elena Vedmedenko — University of Hamburg, Hamburg, Germany

Dirac strings in spin-ices are lines of reversed dipoles joining two quasiparticle excitations. These excitations behave themselves as unbound emergent monopoles if the tension of Dirac strings vanishes. In this work analytical and numerical analysis are used to study dynamics of two-dimensional dipolar spin ices, artificially created analogs of bulk spin-ice, in the regime of bound monopoles. It is shown that in this regime strings rather than monopoles are effective degrees of freedom explaining the finite-width band of Pauling states. A measurable prediction of path-time dependence of endpoints of stretched and then released Dirac string is made and verified via simulations. It is shown that string dynamics is defined by the characteristic tension-to-mass ratio, which is determined by the fine structure constant and lattice dependent parameter. It is proposed to use string tension to achieve spontaneous magnetic currents. A concept of energy storing device on the basis of this principle is proposed and illustrated by an experimental demonstration. A scheme of independent measurement at the nanoscale is proposed.

TT 45.10 Wed 12:00 H32

Spin-orbit torque in antiferromagnets — •Jakub Zelezny[1], Frank Freimuth[2], Yuriy Mokrousov[2], Jacob Gayles[3], Jairo Sinova[3], and Tomas Jungwirth[3] — [1]Institute of Physics of the Czech Academy of Sciences, Czech Republic — [2]Forschungszentrum Julich and JARA, Germany — [3]Institut fur Physik, Johannes Gutenberg Universitat Mainz, Germany

Antiferromagnets are common in nature and just like ferromagnets posses a long-range magnetic order. Unlike ferromagnets though, they have found little practical applications so far, primarily due to their lack of total magnetization. However, development of spintronics opens up ways how they could be used. Antiferromagnets have some advantages over ferromagnets, in particular ultrafast magnetization dynamics and wide range of materials available, including many semiconductors. One of the key problems for application of antiferromagnets in spintronics remains manipulation of the spin-axis. Recently we have predicted that in some bulk antiferromagnets, electrical current can effectively manipulate the magnetic moments [1]. Switching of an antiferromagnet using this method have recently been observed experimentally [2]. The effect is analogous to the spin-orbit torque in ferromagnets. Here we discuss the symmetry of the torques, especially the necessary conditions for their existence and show results of microscopic calculation of the torques in various antiferromagnets.

[1] J. Železný et al., PRL 113 (15), 157201 [2] P. Wadley et al., Science, to be published, arXiv:1503.03765

TT 46: Superconductivity: Fe-based Superconductors - FeSe

Time: Wednesday 10:00–12:45 Location: H19

TT 46.1 Wed 10:00 H19

Superconductivity and electronic structure in single-layer FeSe on $SrTiO_3$ probed by scanning tunneling microscopy — •Jasmin Jandke[1], Jonas Dressner[1], Fang Yang[2], Chunlei Gao[2], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, Karlsruhe Institut of Technology, Germany — [2]Fudan Universität, Shanghai , China

We use high-resoluion scanning tunneling spectroscopy (STS) to study single-layer FeSe on Nb-doped $SrTiO_3$ (001). Features of bosonic excitations were observed in the measured quasiparticle density of states. Furthermore, using STS, quasiparticle interference (QPI) imaging was performed in order to map the multiband electronic structure of FeSe. Compared to previous measurements [1,2], an additional feature is visible in our measured QPI maps on a single-layer FeSe/$SrTiO_3$. The origin of this feature will be discussed.

[1] D. Huang et al. PRL **115**, 017002 (2015)
[2] Q. Fan et al. arXiv:1504.02185 [cond-mat.supr-con] (2015)

TT 46.2 Wed 10:15 H19

High-T_c superconductivity in monolayer FeSe on $SrTiO_3$ via interface-induced small-q electron-phonon coupling — •Alexandros Aperis and Peter M. Oppeneer — Uppsala University, Sweden

A monolayer of FeSe deposited on $SrTiO_3$ becomes superconducting at temperatures that exceed T_c=100 K, as compared to a bulk T_c of 8 K. Recent ARPES measurements have provided strong evidence that an interfaced-induced electron-phonon interaction between FeSe electrons and $SrTiO_3$ phonons plays a decisive role in this phenomenon. However, the mechanism that drives this tantalizing high-T_c boost is still unclear.

Here, we examine the recent experimental findings using fully anisotropic, full bandwidth multiband Eliashberg calculations focusing on the superconducting state of FeSe/STO. We use a realistic ten band tight-binding band structure for the electrons of monolayer FeSe and study how the suggested interface-induced small-q electron-phonon interaction mediates superconductivity. Our calculations produce a high-T_c s-wave superconducting state with the experimentally resolved momentum dependence. Further, we calculate the normal metal/insulator/superconductor tunneling spectrum and identify fin-

gerprints of the interface-induced phonon mechanism.

TT 46.3 Wed 10:30 H19

Tuning orbital-selective correlation effects in the superconducting iron chalcogenides $Rb_{1-x}Fe_{1.6}Se_{2-z}S_z$ — •Zhe Wang[1], Vladimir Tsurkan[1,2], Michael Schmidt[1], Alois Loidl[1], and Joachim Deisenhofer[1] — [1]Experimetal Physics V, University of Augsburg, Augsburg, Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau, Republic of Moldova

We report a terahertz time-domain spectroscopy study on superconducting and metallic iron chalcogenides $Rb_{1-x}Fe_{1.6}Se_{2-z}S_z$ [1,2]. With increasing sulfur doping the superconducting transition is reduced from $T_c = 32$ K for z = 0 and finally suppressed at z = 1.4 [1]. The dielectric constant and the optical conductivity exhibit a metal-to-insulator-type transition associated to an orbital-selective Mott phase [2]. This orbital-selective Mott transition appears at $T_{met} = 90$ K for z = 0 and shifts to higher temperatures for higher doping levels [1], identifying sulfur substitution as an efficient parameter to tune orbital-dependent correlation effects in the iron-chalcogenide superconductors. The reduced correlation strength of the dxy charge carriers may also account for the suppression of the pseudogap-like feature between T_c and T_{met} that was observed for z = 0 [2].

[1] Zhe Wang, V. Tsurkan, A. Loidl, and J. Deisenhofer, arXiv:1506.04614
[2] Zhe Wang, M. Schmidt, J. Fischer, V. Tsurkan, M. Greger, D. Vollhardt, A. Loidl, and J. Deisenhofer, Nature Comm. **5**, 3202 (2014)

TT 46.4 Wed 10:45 H19

Influence of substrate type on transport properties of superconducting $FeSe_{0.5}Te_{0.5}$ thin films — •Feifei Yuan[1,2], Kazumasa Iida[1,3], Marco Langer[1,4], Jens Hänisch[1,4], Ruben Hühne[1], and Ludwig Schultz[1] — [1]IFW, Dresden, Germany — [2]Southeast University, Nanjing, China — [3]Nagoya University, Nagoya, Japan — [4]KIT, Eggenstein-Leopoldshafen, Germany

$FeSe_{0.5}Te_{0.5}$ thin films were grown by pulsed laser deposition on CaF_2, AlO_3 and MgO substrates and structurally and electro-magnetically characterized in order to study the influence of the substrate on their transport properties. The in-plane lattice mismatch between $FeSe_{0.5}Te_{0.5}$ bulk and the substrate shows no influence on the lattice parameters of the films, whereas the type of substrate affects the crystalline quality of the films and, therefore, the superconducting properties. The film on MgO showed an extra peak in the angular dependence of critical current density J_c at $\theta = 180°$ (H//c), which arises from c-axis defects as confirmed by transmission electron microscopy. In contrast, no J_c peaks for H//c were observed in films on CaF_2 and $LaAlO_3$. $J_c(\theta)$ can be scaled successfully for both films without c-axis correlated defects by the anisotropy Ginzburg-Landau approach with appropriate anisotropy ratio γ. The scaling parameter γ is decreasing with decreasing temperature, which is different from what we observed in $FeSe_{0.5}Te_{0.5}$ films on Fe-buffered MgO substrates.

TT 46.5 Wed 11:00 H19

Investigation of the electronic and magnetic structure of thin layer FeTe on Bi_2Te_3 — •Lasse Cornils[1], Sujit Manna[1], Anand Kamlapure[1], Torben Hänke[1], Jin Hu[2], Zhiqiang Mao[2], Bo Brummerstedt Iversen[3], Philip Hofmann[3], Jens Wiebe[1], and Roland Wiesendanger[1] — [1]Department of Physics, University of Hamburg, Hamburg, Germany — [2]Department of Physics, Tulane University, New Orleans, United States — [3]Interdisciplinary Nanoscience Center iNANO, Aarhus University, Denmark

The surprising discovery of Fe based superconductors in 2008 lead to a big effort in finding new materials with very high critical temperatures. One good example are Fe-chalcogenides. Although the parent compound FeTe is not superconducting, the situation changes drastically on interfacing the material with other substrates. Recently He and coworkers [1] found zero resistance at the interface of Bi_2Te_3 films grown on bulk FeTe, which showed a transition temperature of 12K. In this talk we present our latest results on our investigation of the electronic and magnetic nature of epitaxially grown FeTe thin films on the topological insulator Bi_2Te_3 using spin-polarized scanning tunneling microscopy and spectroscopy. Up to several monolayers of FeTe, an antiferromagnetic structure similar to the one observed on its bulk compound FeTe was clearly visible. Surprisingly we found a gap around the Fermi level indicating proximity to superconductivity in coexistence with magnetism on the nanoscale.

[1] Q.-L. He et al., Nature Comm. **5**, 4247 (2014)

15 min. break

Invited Talk TT 46.6 Wed 11:30 H19

On Nematicity, Magnetism and Superconductivity in FeSe — •A. E. Böhmer[1], K. Kothapalli[1], W. T. Jayasekara[1], A. Sapkota[1], U. Kaluarachchi[1], E. I. Timmons[1], P. Das[1], B. G. Ueland[1], G. Drachuck[1], M. Schütt[2], V. Taufour[1], M. A. Tanatar[1], S. L. Bud'ko[1], Y. Xiao[3], R. M. Fernandes[2], R. Prozorov[1], A. I. Goldman[1], and P. C. Canfield[1] — [1]Ames Lab. / Iowa State University, Ames, IA, USA — [2]University of Minnesota, Minneapolis, MN, USA — [3]Argonne National Lab., Argonne, IL, USA

FeSe provides a new perspective on the intensively studied phase interplay in iron-based materials. At ambient pressure, FeSe exhibits the typical (nematic) structural phase transition, but, unusually, no long-range magnetic order and no competition between nematicity and superconductivity. Under pressure, the structural transition is gradually suppressed and a new, likely magnetic phase emerges.

I will present our recent results on the nematic phase and the pressure-temperature phase diagram of vapor-grown single crystals of FeSe. The origin of the nematic resistivity anisotropy at ambient pressure and the pressure evolution of the orthorhombic distortion, the superconducting upper critical field and magnetic ordering are investigated using resistivity, elastoresistivity, diffraction and synchrotron Mössbauer spectroscopy. The relation of magnetism, structure and superconductivity in FeSe will be discussed and compared to other iron-based systems.

Work at Ames Lab. was supported by US DOE, DE-AC02-07CH11358. This research used resources at Argonne National Lab.

TT 46.7 Wed 12:00 H19

Superconductivity and spin excitations in orbitally ordered FeSe — •Andreas Kreisel[1], Shantanu Mukherjee[1,3], Peter J. Hirschfeld[2], and Brian M. Andersen[1] — [1]Niels Bohr Institute, University of Copenhagen, Denmark — [2]University of Florida, Gainesville, FL, USA — [3]Dept. of Physics, State University of New York at Binghamton, Binghamton, NY, USA

We provide a band-structure with low-energy properties consistent with recent photoemission and quantum oscillations measurements on the Fe-based superconductor FeSe[1], including a mean-field like orbital ordering in the d_{xz}/d_{yz} channel, and show that this model also accounts for the temperature dependence of the measured Knight shift and the spin-relaxation rate[2]. An RPA calculation of the dynamical spin susceptibility yields spin excitations which are peaked at wave vector $(\pi, 0)$ in the 1-Fe Brillouin zone, with a broad maximum at energies of order a few meV. Furthermore, the superconducting gap structure obtained from spin fluctuation theory exhibits nodes on the electron pockets, consistent with the 'V'-shaped density of states measured by tunneling spectroscopy on this material. The redistribution of spectral weight in the superconducting state creates a $(\pi, 0)$ "neutron resonance" as seen in recent experiments[3]. Comparing to various experimental results, we give predictions for further studies.

[1] S. Mukherjee *et al.*, PRL **115**, 026402 (2015)
A. Kreisel, *et al.*, arXiv:1506.03593
[2] S.-H. Baek *et al.*, Nat. Mater. **14**, 210 (2015)
A. E. Böhmer *et al.*, PRL **114**, 027001 (2015)
[3] M.C. Rahn *et al.*, PRB **91**, 180501 (2015)
Q. Wang, *et al.*, arXiv:1502.07544

TT 46.8 Wed 12:15 H19

Interplay between iCDW order and electronic excitations in FeSe — •Markus Klug and Joerg Schmalian — Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

The origin of the nematic transition at 90K in FeSe and its underlying mechanism including its relevance for superconductivity remain unknown. Recently, the possibility of imaginary charge density wave order (iCDW), which breaks translational and time reversal symmetry, was proposed [1]. In this talk the implications of iCDW order in elastic neutron scattering and electronic Raman scattering are analyzed. We discuss the emergence of a spin and charge gap as well as the possibility of new collective modes.

[1] A. V. Chubukov, R. M. Fernandes and J. Schmalian, PRB **91**, 201105(R) (2015)

TT 46.9 Wed 12:30 H19

Gap anisotropy in FeSe — •Yevhen Kushnirenko[1], Alexandr Fedorov[1,2], Erik Haubold[1], Bernd Büchner[1], Daniil

Evtushinsky[3], Timur Kim[4], Moritz Hoesch[4], Thomas Wolf[5], 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]Helmholtz-Zentrum Berlin, BESSY, D-12489 Berlin, Germany — [4]Diamond Light Source, Harwell Campus, Didcot, OX11 0DE, United Kingdom — [5]Institut für Festkörperphysik, Karlsruhe Institute for Technology, Karlsruhe 76021, Germany

FeSe is the simplest iron-based superconductor, but details of its electronic structure such as symmetry and structure of the order parameter are still not known. Knowledge of the superconducting gap symmetry can help us to understand mechanism of pairing in this material. We used angle-resolved photoemission spectroscopy (ARPES) for measurements of the superconducting gap. Synchrotron radiation was used as a light source for our experiments. We analyzed a gap behavior in different parts of the three-dimensional Brillouin zone (near Gamma, Z, A and M-point). We have found considerable gap anisotropy on the electron pocket (near A and M-point). The gap anisotropy on the central pocket (near Z-point) is small. Our results put constraints on existing theories of superconductivity in iron-based pnictides and chalcogenides.

TT 47: Correlated Electrons: Other Materials

Time: Wednesday 10:30–13:00 Location: H21

TT 47.1 Wed 10:30 H21

Phonon renormalization in $LaCoO_3$ by inelastic neutron and x-ray scattering — •Maximilian Kauth[1], Frank Weber[1], and John-Paul Castellan[1,2] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie — [2]Laboratoire Léon Brillouin, CEA Saclay

$LaCoO_3$ exhibits two broad magnetic-electric transitions, a diamagnetic to paramagnetic spin-state transition at $T_{SS} \approx 100\,K$ and a metal-insulator transition at $T_{MI} \approx 500\,K$. The spin transitions on heating are proposed to be as follows [1]: from a homogeneous LS state to a mixed Low-Spin/High-Spin (LS/HS) state with strong spin-charge fluctuations at $T=T_{SS}$ and, subsequently, into a homogeneous HS state at $T=T_{MI}$. The lattice participates in the state mixture by expansion of CoO_6 octahedra around the HS sites, while the ones around LS sites have a reduced size [2]. The originally proposed static order [2] has not been observed experimentally and, hence, the ordering is expected to be dynamic and short-ranged. We investigated the lattice dynamical properties of $LaCoO_3$ using inelastic neutron scattering. Based on detailed ab-initio lattice dynamical calculations (performed in our institute), we aim for a comprehensive understanding of lattice dynamics in $LaCoO_3$. The above discussed crossovers and spin state order should be reflected in the lattice degrees of freedom via quasi elastic scattering and phonon renormalization effects.

[1] M. Karolak et al., PRL **115**, 046401 (2015)
[2] J. B. Goodenough, J. Phys. Chem. Solids **6**, 287 (1958)

TT 47.2 Wed 10:45 H21

Excitonic transition in (Pr,Ca)CoO_3 family — •Jan Kuneš and Pavel Augustinský — Insitute of Physics, AS CR, Prague

The members of $(Pr_{1-y}Y_y)_{1-x}Ca_xCoO_3$ family exhibit a continuous phase transition accompanied by disappearance of the fluctuating moment of Co and increase of resistivity by several decades. Most intriguing feature of the low temperature phase is breaking of the time reversal symmetry without presence of ordered atomic moments. We will argue that the experimental observations are explained by condensation of atomic size excitons, which gives rise to ordered magnetic multipoles. We will present model calculations performed with dynamical-mean field theory, which demonstrate general features of the excitonic condensation. In addition, we will present results of material specific LDA+U calculations which uncover the excitonic order in $Pr_{0.5}YCa_{0.5}CoO_3$ and explain its low temperature behavior.

[1] J. Kuneš, P. Augustinský, PRB **90**, 235112 (2014).

TT 47.3 Wed 11:00 H21

Theoretical study of spin-state transition in $LaCoO_3$ using LDA+MLFT — •Evgeny Gorelov[1], Igor Krivenko[2], Michael Karolak[3], and Alexander Lichtenstein[1,2] — [1]European XFEL GmbH Albert-Einstein-Ring 19, 22761 Hamburg, Germany — [2]University of Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany — [3]University of Würzburg, Sanderring 2, 97070 Würzburg, Germany

$LaCoO_3$ demonstrates variety of phase transitions due to competing interactions governing it's electronic structure, including metal-to-insulator transition around T≈500 K and gradual spin-state transition around T≈80-120 K. In this work we focus on spin-state transition, and use theoretical approach of M. Haverkort, taking into account transition metal ion and it's octahedral oxygen surrounding [1]. This approach allow us to calculate the resonant Co $L_{2,3}$ X-ray absorption spectra (XAS), using ab-initio calculated model parameters, i.e. nearest neighbors hopping matrix. The calculations are performed for experimental crystal structures for different temperatures in the range of 5-600 K [2]. In our calculations we include Co 3d orbitals with full Coulomb vertex, and five ligand orbitals, constructed from 2p orbitals of O atoms, forming the octahedra around Co ion. We discuss changes in the XAS spectra induced by thermal expansion of the lattice, as well as caused by change of electron temperature.

[1] M. W. Haverkort, M. Zwierzycki, and O. K. Andersen, PRB **85**, 165113 (2012)
[2] P. G. Radaelli and S.-W Cheong, PRB **66**, 094408 (2002)

TT 47.4 Wed 11:15 H21

Construction of effective low-energy interactions for three-orbital cuprate models with electronic correlation — •Cornelia Hille[1], Xiaodong Cao[2], Carsten Honerkamp[3], Philipp Hansmann[2], and Sabine Andergassen[1] — [1]Institut für Theoretische Physik, Universität Tübingen, Tübingen, Germany — [2]Max Planck Institute for Solid State research, Stuttgart, Germany — [3]Institute for Solid State Theory, RWTH Aachen, Aachen, Germany

Real materials typically have involved bandstructures and a many-body solution of the full Hamiltonian is not feasible. To identify the most relevant degrees of freedom we often start from ab initio single particle (e.g. DFT, Hartree Fock, GW) calculations and integrate out states of high energy remaining with a low-energy effective Hamiltonian. For basically all transition metal oxides this procedure leads to the question if and how to include oxygen 2p states explicitly. We present effective low-energy interactions for three-orbital cuprate models calculated in a cRPA framework. We find effective copper d-state interactions which are strongly dynamically screened by transitions involving the oxygen 2p states.

TT 47.5 Wed 11:30 H21

Self-consistent GW+EDMFT simulation of $SrVO_3$ - Hubbard vs. plasmon physics — •Lewin Boehnke[1], Fredrik Nilsson[2], Ferdi Aryasetiawan[2], and Philipp Werner[1] — [1]University of Fribourg, Switzerland — [2]Lund University, Sweden

$SrVO_3$ has been considered a prototypical strongly correlated metal for more than a decade Its (inverse) photoemission spectra [1] show a characteristic three peak structure close to the Fermi level.

We develop a multi-orbital GW+extended dynamical mean-field theory [2,3] framework, applying approximations of increasing rigor to orbital subsets of increasing degree of correlation with the goal of unbiased finite temperature ab-initio calculations of materials classes with relevant local and non-local many-body correlations.

We use a suitable continuous time quantum Monte Carlo impurity solver (CT-Hyb) [4] to deal with the frequency dependence of the effective impurity interaction and a tailored Matsubara frequency implementation of the GW-algorithm to solve self consistency cycle.

For $SrVO_3$ we find that the screening from nonlocal Coulomb interactions substantially reduces the effective local interaction, suppressing the Hubbard bands. At the same time, plasmon satellites are formed that are consistent with experimental observations. [1]

[1] K. Morikawa, T. Mizokawa, K. Kobayashi, A. Fujimori, H. Eisaki, S. Uchida, F. Iga, and Y. Nishihara, PRB **52**, 13711 (1995)
[2] S. Biermann, F. Aryasetiawan, and A. Georges, PRL **90**, 086402 (2003)
[3] T. Ayral, S. Biermann, and P. Werner, PRB **87**, 125149 (2013)
[4] E. Gull, *et al.* RMP **83**, 349 (2011)

15 min. break

TT 47.6 Wed 12:00 H21

The electronic structure of palladium in the presence of many-body effects — •Andreas Östlin[1,2], Wilhelm Appelt[3,1], Igor di Marco[4], Weiwei Sun[4], Milos Radonjic[1], Michael Sekania[1], Levente Vitos[2,4,5], and Liviu Chioncel[3,1] — [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]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [4]Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75120 Uppsala, Sweden — [5]Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, P.O. Box 49, H-1525 Budapest, Hungary

Including on-site electronic interactions described by the multi-orbital Hubbard model we study the correlation effects in the electronic structure of bulk palladium within the framework of combined density functional and dynamical mean field theory, DFT+DMFT, using the fluctuation exchange approximation. The agreement between the experimentally determined and the theoretical lattice constant and bulk modulus is improved when correlation effects are included. At the same time we discuss the possibility of satellite formation in the high energy binding region. Investigation of non-local correlation effects within the *GW* method is also performed.

TT 47.7 Wed 12:15 H21

Phase separation in $Y_{0.63}Ca_{0.37}TiO_3$ — •Thomas Koethe[1], Bernhard Zimmer[1], Raphael German[1], Alexei Barinov[2], Alexander Komarek[1,3], Fulvio Parmigiani[2], Markus Braden[1], and Paul van Loosdrecht[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Elettra Sincrotrone, Trieste (Italy) — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

We have investigated the domain structure and Raman response of $Y_{0.63}Ca_{0.37}TiO_3$ single crystals which show a clear metal-to-insulator transition at ca. 170 K, with a wide hysteresis in the resistivity ranging down to ca. 50 K. We observe by use of a conventional optical microscope the appearance of two distinct regions at temperatures below ca. 200 K, with a characteristic length scale of order of 10 μm. By means of Raman spectroscopy we can identify the regions to correspond to the metallic and insulating domains, and follow the evolution of the domains as function of temperature down to 5 K. Preliminary results of spacially resolved PES confirm the presence of electronically distinct regions on the μm scale at low temperature.

TT 47.8 Wed 12:30 H21

Breathing Mode Distortion and Magnetic Order in Rare-Earth Nickelates RNiO$_3$ — •Alexander Hampel and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

Rare-earth nickelate perovskites display a rich and not yet fully understood phase diagram, where all RNiO$_3$ compounds with R from Sm to Lu undergo a non-magnetic metal-insulator transition (MIT). This transition is connected to a lattice distortion, which can be described as breathing mode of the oxygen octahedra surrounding the Ni cations. Between 100-250 K the RNiO$_3$ compounds undergo a magnetic transition to an antiferromagnetic (AFM) state, with a wavevector $k = \left[\frac{1}{4}\frac{1}{4}\frac{1}{4}\right]$ relative to the underlying simple cubic perovskite structure.
Here, we use density functional theory and its extensions (DFT+U, DFT+DMFT) together with distortion mode analysis to explore the interplay between lattice distortions, magnetic order, and the strength of the local Coulomb interaction U in rare earth nickelates. Our results show a strong dependency of the breathing mode amplitude on the magnetic order, with a much larger breathing mode obtained for the AFM state compared to the ferromagnetic case. Furthermore, we demonstrate that DFT+U is able to capture the correct trends of the lattice distortions across the nickelate series.

TT 47.9 Wed 12:45 H21

Metal-insulator transition in 2D antiferromagnet $FePS_3$ upon applied pressure — •Matthew John Coak[1], Charles Robert Sebastian Haines[1,2], and Siddarth Shankar Saxena[1] — [1]Cavendish Laboratory, University of Cambridge — [2]CamCool Research Ltd, UK

$FePS_3$ belongs to a rich family of structurally and magnetically quasi-two-dimensional compounds, with a magnetic ground state in which spins are ordered as ferromagnetic chains coupled antiferromagnetically. At ambient pressure, it is an insulator with a direct gap of approximately 0.5 eV and a room temperature resistivity of approximately 104 Ωcm.

We present the results of resistivity measurements under pressures up to 110 kbar for this material. The insulating phase is suppressed at a pressure in the range 40-70 kbar giving way to a new metallic phase. Interesting intermediate behaviour is seen at pressures around the transition as the gap closes. At high pressure, the resistivity develops linear temperature dependence with an upturn in resistivity which may indicate a low temperature phase transition or impurity scattering.

TT 48: Frontiers of Electronic Structure Theory: Focus on Topology and Transport II (Joint session of DS, HL, MA, MM, O and TT organized by O)

Time: Wednesday 10:30–13:00 Location: H24

TT 48.1 Wed 10:30 H24

Coupled-Cluster approach for both molecules and solids in the numeric atom-center orbital framework — •Tonghao Shen, Arvid Conrad Ihrig, Igor Ying Zhang, and Matthias Scheffler — *Fritz-Haber-Institut der MPG, Berlin.*

For a quantitative prediction of material properties, an advanced description of electronic correlation is crucial. As the "gold standard" correlation method in quantum chemistry, the coupled-cluster (CC) ansatz with singles, doubles and perturbative triples (CCSD(T)) is starting to gain attention in materials science[1]. At present, the CCSD(T)-quality description of the correlation effects in solids can be achieved by either studying the cluster-size convergence toward the bulk in real space[1] or implementing CCSD(T) for extended systems in reciprocal space[2]. In order to investigate and compare these approaches on an equal footing, it is essential to have a computational platform that enables CCSD(T) simulations to be carried out using both cluster and periodic models in a single computational environment. In this report, we present a CCSD(T) implementation for both molecules and solids in the all-electron full-potential code FHI-aims[3] with numeric atom-center orbital(NAO) basis sets. A special memory-distribution strategy is designed to significantly reduce the inter-CPU communication, which is the main challenge for the parallelization of wave-function methods. The accuracy and efficiency are demonstrated for a group of molecules, 1D-, 2D- and 3D-periodic materials. [1] C. Müller, *et al.*, PCCP. **14**, 7605 (2012); [2] A. Grüneis, *et al.*, JCTC **7**, 2780 (2011); [3] V. Blum, *et al.*, CPC **180**, 2175-2196 (2009).

TT 48.2 Wed 10:45 H24

Surface adsorption energetics at the "gold standard": Small molecule binding to TiO_2(110) — •Daniel Berger[1,2], A. Kubas[3], D. Manganas[3], H. Oberhofer[1], F. Neese[3], and K. Reuter[1] — [1]TU München — [2]University of California, Los Angeles — [3]MPI für chemische Energiekonversion, Mülheim an der Ruhr

Adsorption energies at oxide surfaces are central quantities required for catalysis, energy and a multitude of other application areas. At present, the by far dominant computational method to obtain such energetics is density-functional theory (DFT). Unfortunately, systematic benchmarking of such energetics against accurate reference numbers from correlated wave-function theory as known from molecular systems is scarce, largely owing to the fact that the latter techniques are often not available for standard periodic boundary condition supercell calculations.

We address this situation with a solid-state QM/MM embedded cluster approach, in which the adsorbate and immediate surrounding surface atoms are described quantum mechanically, while the long-range electrostatic interactions are accounted for through a polarizable force

field. This yields a numerically highly efficient approach that enables use of the recently developed domain-based local pair natural orbital coupled cluster method with single-, double- and perturbative triple-excitations (DLPNO-CCSD(T)) in the quantum region. We exploit corresponding "gold standard" adsorption energies for a set of prototypical small molecules interacting with the rutile TiO_2(110) surface for a systematic benchmark of DFT numbers.

TT 48.3 Wed 11:00 H24

Water adsortpion on surfaces form many-body perturbation theory — •Theodoros Tsatsoulis and Andreas Grüneis — Max-Planck-Institute for Solid State Research, Stuttgart

The accurate description of the interaction of molecules with surfaces is of crucial importance for a wide range of phenomena. While Kohn-Sham density functional theory is one of the most widely-used methods for describing the electronic structure of surfaces, many local and semi-local functionals are often not able to produce accurate molecular adsorption energies. Quantum chemical wave-function based methods such as Møller-Plesset perturbation theory (MP2) and coupled-cluster methods promise controllable accuracy, however, at much higher computational costs. Large part of the latter is due to the number of virtual states. We consider an approach whereby the occupied orbitals are converged in a plane wave basis, whereas the virtual space is then constructed using pseudized Gaussian orbitals expanded in plane waves, leading to reduced computational cost. In particular we study water adsorption on bulk LiH and h-BN sheets at the level of MP2 theory within the projector-augmented-wave method as implemented in VASP [1]. The results are compared to state-of-the-art methods such as hybrid functionals and diffusion Monte Carlo [2].

[1] Marsman et al., The Journal of Chemical Physics, 130, 184103 (2009)

[2] Al-Hamdani et al., The Journal of Chemical Physics, 142, 181101 (2015)

TT 48.4 Wed 11:15 H24

Photo-isomerization in azobenzene-functionalized self-assembled monolayers: The impact of many-body effects — •Caterina Cocchi and Claudia Draxl — Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Self-assembled monolayers (SAMs) of azobenzene-functionalized alkanethiols on gold suffer from hindered photo-isomerization, as observed experimentally [1]. While this behavior is generally ascribed to strong intermolecular coupling, a clear microscopic understanding of this phenomenon is still missing. In order to address this question, we perform a first-principles study of the excited-state properties of azobenzene-functionalized SAMs. In the framework of many-body perturbation theory (GW approximation and Bethe-Salpeter equation), as implemented in the all-electron full-potential code exciting [2], we investigate the optical absorption spectra of these materials, inspecting the influence of packing density and functionalization of the azobenzene molecules with different end groups. Through a systematic analysis of the character of the excitations, we clarify the role and interplay of screening and local-field effects, which strongly impact light absorption and hence photo-isomerization in these systems.

[1] C. Gahl et al. J. Am. Chem. Soc. 132, 1838 (2010). [2] A. Gulans et al. J. Phys.: Condens. Matter 26, 363202 (2014).

TT 48.5 Wed 11:30 H24

Laplace-transformed MP2 with localized Resolution of Identity -efficient in-memory MP2 for large systems — •Arvid Conrad Ihrig[1], Patrick Rinke[2], Igor Ying Zhang[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Aalto University, Helsinki, Finland

A well-known problem in local and semi-local density functional approximations and to a lesser extend also in hybrid functionals is the one-electron self-interaction error, which can lead to a qualitatively wrong description for applications like charge-transfer systems. One possible remedy is the 2nd order Møller-Plesset perturbation theory (MP2), which does not suffer from this error. However, the time and memory requirements for MP2 prevent it routine-use for large molecular and periodic systems. The Laplace-transformed MP2 (LT-MP2) [1] can significantly reduce the computational time, but requires the usage of intermediate variables stored on disk, resulting in an inefficient usage of computational resources. In this work we combine the LT-MP2 with our localized Resolution of Identity (RI-LVL) [2] approach to eliminate the disk-storage bottleneck and fully exploit massive parallelization strategies. RI-LVL expands the basis function pairs in the electron repulsion integrals in local auxiliary basis sets. For the example of water clusters, we demonstrate the favourable memory scaling (at worst N^2) of our new MP2 implementation, which facilitates the in-memory calculation of large systems at high accuracies.

[1] P. Ayala et al., J. Chem. Phys. 110, 3660 (1999)
[2] Ihrig et al., New J. Phys. 17, 093020 (2015)

TT 48.6 Wed 11:45 H24

GW **singles contributions for the random phase approximation correlation energies** — •Jiri Klimes[1], Merzuk Kaltak[2], Emanuele Maggio[3], and Georg Kresse[3] — [1]J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic — [2]Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY — [3]University of Vienna, Faculty of Physics, Vienna, Austria

The random phase approximation (RPA) to the correlation energy yields often very accurate results for condensed matter systems. However, a general tendency to underbind has been observed for systems such as molecular solids or for adsorption. One of the ways that have been proposed to improve the accuracy of RPA are the so-called singles corrections of Ren and coworkers [1]. We present our derivation of the singles corrections using the assumption that the electron density changes when going from the reference to the interacting system [2]. This leads to a very compact expression for the corrections. Moreover, the singles formula can be easily modified to account for screening effects, giving the *GW* singles. We assess the effect of both the original and modified singles on covalently and metallically bonded systems as well as on simple weakly bonded systems. Finally, we show that adding the singles corrections leads to considerably improved adsorption energies and lattice energies of molecular solids.

[1] Ren, Tkatchenko, Rinke, Scheffler, Phys. Rev. Lett **106**, 153003 (2010).

[2] Klimeš, Kaltak, Maggio, Kresse, J. Chem. Phys. **143**, 102816 (2015).

TT 48.7 Wed 12:00 H24

Long-range corrected DFT meets *GW*: Vibrationally resolved photoelectron spectra from first principles — •Thomas Körzdörfer — Institut für Chemie, Universität Potsdam, D-14476 Potsdam

We introduce an entirely non-empirical and computationally efficient scheme to calculate highly reliable vibrationally resolved photoelectron spectra for molecules from first principles.[1] To this end, we combine non-empirically tuned long-range corrected hybrid functionals with non-self-consistent many-body perturbation theory in the G_0W_0 approximation and a Franck-Condon multi-mode analysis based on DFT-calculated frequencies. The vibrational analysis allows for a direct comparison of the GW-calculated spectra to gas-phase ultraviolet photoelectron measurements of neutral and anionic molecules, respectively. In addition, vertical IPs and EAs were benchmarked against other *GW* methods and basis-set extrapolated CCSD(T) results for a recently introduced test set of 24 molecules frequently used in organic electronics.[2] G_0W_0@LRC-DFT yields mean absolute errors on the order of 0.1 eV for IPs, EAs, and fundamental gaps, clearly outperforming commonly used G_0W_0 approaches as well as partially and fully self-consistent *GW* methods.

[1] L. Gallandi and T. Körzdörfer, JCTC **11**, 5391 (2015).
[2] L. Gallandi, N. Marom, P. Rinke, and T. Körzdörfer, JCTC *accepted for publication* (2015).

TT 48.8 Wed 12:15 H24

LDA-1/2 as a starting point for G_0W_0 calculations — •Ronaldo Rodrigues Pela[1,2], Ute Werner[1], Dmitrii Nabok[1], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany — [2]Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil

For many semiconductors and insulators, LDA represents a bad starting point for G_0W_0 calculations. Hybrid functionals improve upon LDA, but at the price of increasing computational cost of about 2 orders of magnitude. An alternative starting-point for the single-shot G_0W_0 can be the LDA-1/2 method [1], because it approximately includes the self-energy of quasi-particles within a generalized Kohn-Sham scheme, leading to improved band-gaps over the LDA ones, but without being computationally more involved. In this work, we systematically compare 3 starting-points for G_0W_0 calculations: LDA, PBE0, and the LDA-1/2 method. A selection of semiconductors (C, Si, SiC, AlP, LiF, MgO, Ne, Ar, GaN, GaAs, CdS, ZnS, and ZnO) is chosen for this benchmark. We demonstrate that LDA-1/2 is a good

choice in most cases, reducing the root mean square error in band-gap predictions by 50% when compared to G_0W_0 on top of LDA or PBE0. With the exception of large band gap materials, LDA-1/2 predictions are already close to the experimental band gaps, and thus G_0W_0 has minor effects.

Reference [1]: Phys. Rev. B 78, 125116 (2008).

Acknowledgements: "Coordenação de Aperfeiçoamento de Pessoal de Nível Superior" (CAPES) and "Alexander von Humboldt Stiftung".

TT 48.9 Wed 12:30 H24

DFT+U within a numeric atom-centered orbital basis — •Matthias Kick, Harald Oberhofer, and Karsten Reuter — Technische Universität München

Materials like transition metal oxides (TMOs) still challenge a description through first-principles density-functional theory (DFT). Appropriately capturing the electron localization in TMOs generally requires at least hybrid exchange-correlation functionals. Such higher-rung functionals come with appreciable computational cost, which limits their use in large supercell calculations. For such applications effective and numerically less intense approaches are therefore still a much sought alternative.

One such method is the DFT+U approach, where the on-site Coulomb correlation effects are treated using a model Hamiltonian, while remaining interactions are treated on the level of semi-local DFT. Full DFT+U functionality including nuclear gradients (forces) has been implemented in the electronic structure code *FHI-aims*. We account for three common occupation matrix representations, differing in the way how the occupations of the correlated subspaces are determined. We critically discuss their performance and differences in the context of the numeric atomic orbital basis sets employed in *FHI-aims*.

The established numerically efficient framework is finally used to address neutral and charged oxygen vacancies at the $TiO_2(110)$ surface within a solid-state embedding approach.

TT 48.10 Wed 12:45 H24

High-throughput Screening and Statistical Learning for Design of Transparent Conducting Oxides — •Christopher Sutton, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft

Transparent conducting oxides (TCOs) represent a class of well-developed and commercialized wide-bandgap semiconductors that are crucial for many electronic devices. Ternary Al, Ga, and In-based sesquioxides are investigated as alternative wide-bandgap semiconductors motivated by very intriguing recent experimental work that has demonstrated bandgap engineering in (GayIn1-y)2O3 from 3.8 eV to ca. 5 eV[1] and ca. 5 eV to 7.5 eV for (Al1-xGax)2O3.[2]

New ternary oxides with the chemical structure of (AlxGayIn1-x-y)2O3 have been identified using cluster expansion (CE) models combined with fast stochastic optimization techniques (e.g., Wang-Landau and diffusive nested sampling) in order to efficiently search potential (ordered and disordered) configurations within a given lattice and for different temperatures. Wang-Landau and diffusive nested sampling has also allowed for a consideration of the effect of entropy on the relative stability of ternary oxides. Statistical learning has also been used to identify a structure-property relationship to efficiently identify new wide-band gap TCOs to improve the fundamental chemical and physical properties (e.g., conductivities, mobilities, and optical transparency) by investigating the parameters that control these properties.

[1] F Zhang, et al., Solid State Communications 2014, 186, 28. [2] H Ito, et al., Japanese Journal of Applied Physics 2012, 51, 100207.

TT 49: Symposium on Quantum Signatures in Magnetism (SYQS) (Joint symposium of HL, MA, O and TT organized by MA)

Time: Wednesday 15:00–17:45 Location: H1

Invited Talk TT 49.1 Wed 15:00 H1

Magnonic macroscopic quantum states and supercurrents — •Burkard Hillebrands[1], Dmytro A. Bozhko[1,2], and Alexander A. Serga[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, Germany

Magnons, the quanta of spin waves, are bosons and can form a Bose-Einstein condensate (BEC) - a spontaneous coherent ground state - established independently of the magnon excitation mechanism. The magnon BEC has zero group velocity and, thus, cannot be directly used for information transport. However, a collective motion of condensed magnons driven by a phase gradient in the condensate wavefunction - a magnon supercurrent - is a most promising candidate for the utilization of magnon macroscopic quantum phenomena at room temperature for spin information transport and processing. We report experimental evidence for the generation of a magnonic supercurrent obtained using Brillouin light scattering experiments. Here the phase gradient is induced by a thermal gradient. A rate equation model describes the experimental findings very well. Several other means to generate the needed gradient of the phase of the condensate wave function will be discussed. The work is supported by the DFG within the SFB/TR 49.

Invited Talk TT 49.2 Wed 15:30 H1

Elementary excitations of magnetic insulators and its heterostructures with metals — •Gerrit Bauer — Institute for Materials Research, Tohoku University, Sendai, Japan

Magnetic insulators such as yttrium iron garnet (YIG) are prime candidates for the search of quantum signatures in magnetism due to their superiors magnetic quality. Metal contacts to magnetic insulators are a possible route to observe them electrically.

In this talk I will review the knowledge about the elementary excitations of magnetic insulators, i.e., magnons, magnon-polarons and magnon-polaritons, as well as their coupling to metal contacts. While to date most experiments can be explained by semiclassical concepts, these excitations offer a route to observe up to now elusive quantum effects.

Invited Talk TT 49.3 Wed 16:00 H1

Cavity Spintronics — •Can-Ming Hu — Department of Physics and Astronomy, University of Manitoba, Winnipeg, Canada R3T 2N2

Strong coupling between magnons and microwave photons has recently been theoretically proposed [1] and experimentally investigated using both microwave transmission [2-4] and electrical detection methods [5]. These works build the foundation for the emerging field of Cavity Spintronics [6], where the development of spintronics merges with the advancement in cavity quantum electrodynamics and cavity polaritons, thereby creating new theoretical and experimental avenues for studying wave physics, developing quantum technology, and facilitating spintronics applications.

Based on the remarkable achievements of the pioneers of Cavity Spintronics, this talk aims to provide a brief introduction of this exciting new frontier of condensed matter research to colleagues working on magnetism, spintronics, and microwave technologies. Related work recently done by our group at the University of Manitoba will be reported [5-8].

[1] Ö. O. Soykal et al., Phys. Rev. Lett. 104, 077202 (2010). [2] H. Huebl, et al., Phys. Rev. Lett. 111, 127003 (2013). [3] Y. Tabuchi, et al., Phys. Rev. Lett. 113, 083603 (2014). [4] X. Zhang, et al., Phys. Rev. Lett. 113, 156401 (2014). [5] L.H Bai, et al., Phys. Rev. Lett. 114, 227201 (2015). [6] C.-M. Hu, arXiv: 1508.01966. [7] B.M. Yao, et al., Phys. Rev. B, 92, 184407 (2015). [8] For more information, please check: http://www.physics.umanitoba.ca/~hu/

15 min. break

Invited Talk TT 49.4 Wed 16:45 H1

Hybrid Quantum Systems - Coupling Color Centers to Superconducting Cavities — •Johannes Majer — TU Wien / Atominstitut

Hybrid quantum systems based on spin-ensembles coupled to superconducting microwave cavities are promising candidates for robust experiments in cavity quantum electrodynamics (QED) and for future technologies employing quantum mechanical effects. The main source of decoherence in this systems is inhomogeneous dipolar spin broadening and a full understanding of the complex dynamics is essential and has not been addressed in recent studies yet. We investigate the

influence of a non-Lorentzian spectral spin distribution in the strong coupling regime of cavity QED. We show for the first time experimentally how the so-called cavity protection effect influences the decay rate of coherent Rabi oscillation by varying the coupling strength in our experiment. We then demonstrate how the Rabi oscillation amplitude can be enhanced by two orders of magnitude by pulsing the strongly coupled system matching a special resonance condition. Giving a way improving the coherent manipulation of the spin polarization helping to improve fidelity and performance in hybrid quantum systems.

Invited Talk TT 49.5 Wed 17:15 H1

Quantum enhanced sensing with single spins in diamond — •Fedor Jelezko — Institute of Quantum Optics, Ulm University

I will discuss recent developments transforming quantum control tools into quantum technologies based on single nitrogen-vacancy (NV) centers in diamond. I will present ultrasensitive MRI at nanoscale and recently developed magnetometry protocols that use quantum error correction as a resource. Experiments with novel colour centers including silicon-vacancy (SiV) will also be presented.

TT 50: Correlated Electrons: Frustrated Magnets - Theory

Time: Wednesday 15:00–19:15 Location: H18

TT 50.1 Wed 15:00 H18

Thermal conductivity of the Kitaev spin ladder — •Wolfram Brenig and Alexandros Metavitsiadis — Institute for Theoretical Physics, Technical University Braunschweig, Germany

We analyze the thermal conductivity of the Kitaev spin model on a two leg ladder, 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. The results will be contrasted against known thermal conductivities of other integrable spin models. Speculations on the impact of including an additional isotropic Heisenberg exchange will be made.

TT 50.2 Wed 15:15 H18

Classification of gapless Z_2 spin liquids in three-dimensional Kitaev models — •Kevin O'Brien, Maria Hermanns, and Simon Trebst — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

The formation of spin liquids in frustrated quantum magnets makes for an exciting prospect due to their hosting fractionalized excitations and emergent gauge fields. Unfortunately, they are notoriously difficult to study as there are often no good analytical methods available and Quantum Monte Carlo simulations are hindered by the infamous sign problem. The Kitaev honeycomb model is a notable exception of a frustrated spin model which is exactly solvable and which hosts a number of distinct quantum spin liquid ground states. As such, it allows for a rare opportunity to study the physics of spin liquids with full analytical tractability.

Here we study the fractionalization of magnetic moments into Majorana fermions and a Z_2 gauge field in a generalization of the Kitaev honeycomb model to a number of three-dimensional, tricoordinated lattices. While the excitations of the gauge field are always gapped, the Majorana fermions may form a gapless dispersion with either topologically protected Weyl nodes, symmetry protected nodal lines, or full 2D Fermi surfaces. We show that the nature of these Majorana (semi)metals can be deduced from an elementary analysis of the projective time-reversal and inversion symmetries for a given lattice, allowing us to classify the gapless spin liquids of three-dimensional Kitaev models.

TT 50.3 Wed 15:30 H18

Detailed phase diagram of Kitaev-Heisenberg model — •Dorota Gotfryd[1,2], Juraj Rusnacko[3], Jiri Chaloupka[3], and Andrzej M. Oles[2,4] — [1]Institute of Theoretical Physics, University of Warsaw, Poland — [2]Marian Smoluchowski Institute of Physics, Jagellonian University, Poland — [3]Central European Institute of Technology, Masaryk University, Czech Republic — [4]Max-Planck-Institut FKF, Germany

We present detailed phase diagram for the Kitaev-Heisenberg (KH) model [1] obtained by two approaches: ED and ED with cluster mean field introduced in [2]. While the evolution of ordered moments resulting from second method allows for more direct order/disorder phase transition analysis – we deliberately break SU(2) symmetry, spin correlation functions, spin-structure factor and dynamical spin susceptibility obtained from ED provide more details about the nature of two distinct spin liquid regions.

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

[1] J. Chaloupka and G. Khaliullin, PRB **92**, 043032 (2015)
[2] A. F. Albuquerque et al., PRB **84**, 024406 (2011).

TT 50.4 Wed 15:45 H18

Quantum disordered insulating phase in the frustrated cubic-lattice Hubbard model — •Stephan Rachel[1], Manuel Laubach[1,2], Darshan Joshi[1], Johannes Reuther[3], Ronny Thomale[2], and Matthias Vojta[1] — [1]TU Dresden, Institut für Theoretische Physik — [2]Universität Würzburg, Institut für Theoretische Physik — [3]FU Berlin & Helmholtz-Zentrum Berlin

In the quest for quantum spin liquids in three spatial dimensions (3D), we study the half-filled Hubbard model on the simple cubic lattice with hopping processes up to third neighbors. Employing the variational cluster approach (VCA), we determine the zero-temperature phase diagram: In addition to a paramagnetic metal at small interaction strength U and various antiferromagnetic insulators at large U, we find an intermediate-U antiferromagnetic metal. Most interestingly, we also identify a non-magnetic insulating region, extending from intermediate to strong U. Using VCA results in the large-U limit, we establish the phase diagram of the corresponding J_1–J_2–J_3 Heisenberg model. This is qualitatively confirmed – including the non-magnetic region – using spin-wave theory. Further analysis reveals a striking similarity to the behavior of the J_1–J_2 square-lattice Heisenberg model, suggesting that the non-magnetic region hosts a 3D spin-liquid phase.

TT 50.5 Wed 16:00 H18

Quantum paramagnet in the Heisenberg model on the cubic lattice: a case study of a novel method for three-dimensional quantum magnetism — •Yasir Iqbal[1], Stephan Rachel[2], Ronny Thomale[1], and Johannes Reuther[3,4] — [1]Institute for Theoretical Physics and Astrophysics, Julius-Maximilian's University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute for Theoretical Physics, Technische Universität Dresden, D-01062 Dresden, Germany — [3]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, D-14195 Berlin, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany

A holy grail in quantum magnetism is the search for quantum spin liquids in strongly correlated systems. In particular, $2D$ quantum spin systems have been convincingly shown, both experimentally and theoretically, to host spin liquids. In contrast to $2D$, where there are by now powerful numerical methods available, the case of $3D$ remains out of reach of most numerical methods, or restricted to very small systems. We discuss recent developments of the pseudo-fermion functional renormalization group (PF-FRG) method enabling an efficient study of $3D$ systems. We use this framework to investigate the spin-1/2 quantum Heisenberg $J_1 - J_2 - J_3$ antiferromagnetic model on the simple cubic lattice, and obtain the phase diagram, which reveals the existence of a quantum paramagnetic phase over an extended region in parameter space, with a featureless spin susceptibility profile. A state-of-the-art implementation enables simulation of very large systems

15 min. break

TT 50.6 Wed 16:30 H18

Finite temperature dynamics of spin-1/2 chains with symmetry breaking interactions — Alexander C. Tiegel[1], •Salvatore R. Manmana[1], Thomas Pruschke[1], and Andreas Honecker[2] — [1]Institut f. Theor. Physik, Univ. Göttingen, 37077 Göttingen —

[2]LPTM, Université de Cergy-Pontoise, France

I will discuss recent developments for flexible matrix product state (MPS) approaches to calculate finite-temperature spectral functions of low-dimensional strongly correlated quantum systems. The main focus will be on a Liouvillian formulation [1]. The resulting algorithm does not specifically depend on the MPS formulation, but is applicable for any wave function based approach which can provide a purification of the density matrix, opening the way for further developments of numerical methods. Based on MPS results for various spin chains, in particular systems with Dzyaloshinskii-Moriya interactions caused by spin-orbit coupling and dimerized chains, I will discuss how symmetry breaking interactions change the nature of the finite-temperature dynamic spin structure factor obtained in ESR [2] and neutron scattering experiments.

[1] A.C. Tiegel et al., PRB **90**, 060406(R) (2014)
[2] A.C. Tiegel et al., arXiv:1511.07880 (submitted to PRB)

TT 50.7 Wed 16:45 H18

Quantum Monte Carlo in the spin dimer-basis — •Jonas Stapmanns[1], Andreas Honecker[2], and Stefan Wessel[1] — [1]Institute for Theoretical Solid State Physics RWTH Aachen University, Aachen, Germany — [2]Laboratoire de Physique Théorique et Modélisation Université de Cergy-Pontoise, Pontoise, France

Quantum Monte Carlo simulations of frustrated spin systems are usually plagued by a severe sign-problem. However, due to its dependence on the employed computational basis, it can be feasible to reduce or even avoid the sign-problem by an appropriate local basis choice. Here, we consider in particular the possibility of simulating dimerized quantum spin systems based on a spin dimer-basis formulation of the stochastic series expansion algorithm. We discuss this simulation scheme and present results for thermodynamic properties of the fully-frustrated spin-1/2 Heisenberg ladder as well as for the fully-frustrated square lattice bilayer Heisenberg model.

TT 50.8 Wed 17:00 H18

Phase diagram of frustrated spin ladders with ring exchange interaction — •Alexandros Metavitsiadis[1] and Sebastian Eggert[2] — [1]Institute for Theoretical Physics, Technical University Braunschweig, Germany — [2]Physics Department and Research Center OPTIMAS, Technical University of Kaiserslautern, Germany

The ground state properties of spin ladders are studied, emphasizing the role of frustration. We present a unified field theory calculation for ladders with different geometries and using the renormalization group we deduce their phase diagrams in the presence of in-chain next nearest neighbor interactions as well as plaquette ring exchange interactions. We find the magnetically ordered states, Haldane and rung singlet, in addition to dimerized patterns, columnar dimer and staggered dimer. Lastly, we show that the interplay of the larger unit cell and the ring exchange interaction induces a ferro-antiferromagnetic state, otherwise expected at much higher energy scales.

TT 50.9 Wed 17:15 H18

The infinite-PEPS algorithm: improvements, and its application to spin-S Kagome quantum antiferromagnets in a field — •Roman Orus[1], Phien Ho[2], Johann Bengua[2], Hoang Tuan[2], Philippe Corboz[3], Thibaut Picot[4], Marc Ziegler[1], and Didier Poilblanc[4] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]University of Technology Sydney, Sydney 2007, Australia — [3]Institute for Theoretical Physics, University of Amsterdam, Science Park 904 Postbus 94485, 1090 GL Amsterdam, The Netherlands — [4]Laboratoire de Physique Theorique, IRSAMC, CNRS and Université de Toulouse, UPS, F-31062 Toulouse, France

The infinite Projected Entangled Pair States (iPEPS) algorithm has become a useful tool in the calculation of ground state properties of 2d quantum lattice systems in the thermodynamic limit. Here I will present results concerning iPEPS in two directions. In the first part of my talk I will explain how to overcome some of the current limitations of the method by using a gauge fixing and a "fast full update" of the tensors, implying dramatic computational savings, and improved overall stability. In the second part, I will explain how the method can be applied to obtain the phase diagrams of Spin-S Heisenberg quantum antiferromagnets on the Kagome lattice, up to S = 2.

TT 50.10 Wed 17:30 H18

Application of the DMRG in two dimensions: a parallel tempering algorithm — •Shijie Hu[1], Jize Zhao[2], Axel Pelster[1], Xuefeng Zhang[1], and Sebastian Eggert[1] — [1]Department of Physics and Research Center Optimas, Technical University Kaiserslautern, 67663 Kaiser- slautern, Germany — [2]Institute of Applied Physics and Computational Mathematics, Beijing 100088, China

The Density Matrix Renormalization Group (DMRG) is known to be a powerful algorithm for treating one-dimensional systems. When the DMRG is applied in two dimensions, however, the convergence becomes much less reliable and typically "metastable states" may appear, which are unfortunately quite robust even when keeping a very high number of DMRG states. To overcome this problem we have now successfully developed a parallel tempering DMRG algorithm. Similar to parallel tempering in quantum Monte Carlo, this algorithm allows the systematic switching of DMRG states between different model parameters, which is very efficient for solving convergence problems. Using this method we have figured out the phase diagram of the xxz model on the anisotropic triangular lattice which can be realized by hardcore bosons in optical lattices.

15 min. break

TT 50.11 Wed 18:00 H18

Heisenberg antiferromagnets on the hexagonal bilayer with interlayer frustration — •Boris Celan and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig

Frustrated single layer Heisenberg antiferromagnets on the hexagonal lattice have seen an upsurge of interest. Recently also a bilayer system, i.e. $Bi_3Mn_4O_{12}(NO_3)$, with possibly interlayer frustration has come under scrutiny. For this material $S = 3/2$, rendering spin wave analysis a viable approach. We present results of a selfconsistent spin wave calculation for the hexagonal Heisenberg bilayer up to second order in $1/S$, explicitly taking into account the impact of interlayer frustration. Findings for the quantum phase diagram, the local moments, the ground state energies, and the magnon dispersions versus the exchange interactions will be discussed. Our results will be contrasted against those obtained from methods applied to the quantum limit $S = 1/2$.

TT 50.12 Wed 18:15 H18

Coulomb spin liquid on the honeycomb lattice — •Jorge Armando Rehn[1], Arnab Sen[2], Kedar Damle[3], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Indian Association for the Cultivation of Science, Kolkata, India — [3]Tata Institute of Fundamental Research, Mumbai, India

This talk will present a study of the maximally frustrated classical Heisenberg model on the honeycomb lattice which displays a Coulomb spin liquid phase of a new kind, where emergent gauge charges live on a triangular lattice, and, upon dilution with non-magnetic impurities, this model exhibits new fractionalized objects carrying 1/3 of the moment of the original spins. A zero temperature effective theory for these fractionalized, Coulomb vector charges, will be presented, which represents a new kind of Coulomb spin model presenting a glassy phase.

TT 50.13 Wed 18:30 H18

Kagome spin liquid: a deconfined critical phase driven by the gauge fluctuation — •Yin-Chen He[1], Fuji Yohei[1], and Subhro Bhattacharjee[2] — [1]Max-Planck-Institut fur Physik komplexer Systeme — [2]International Centre for Theoretical Sciences, Tata Institute of Fundamental Research

Recently, new insights emerge into the celebrated problem of spin liquids on the kagome lattice: The kagome spin liquid, the ground state of the nearest neighbor Heisenberg model, survives under the extreme easy-axis anisotropy, and it is neighboring a chiral spin liquid phase. Motivated by this, we study the kagome spin liquid problem in the easy-axis limit, and reformulate it to a lattice gauge model. In this framework, we propose a new theory that, the parent state of the kagome spin liquid is a deconfined critical point, which under the $U(1)$ gauge fluctuation gets extended into a critical phase. Besides the novelty, our theory also makes a vital connection between the seemly different subjects: topological order, critical spin liquid, symmetry protected topological phase, and deconfined criticality.

TT 50.14 Wed 18:45 H18

The transverse field Ising model on the three dimensional swedenborgite lattice: Disorder-by-disorder and an effective classical two dimensional dimer model — •Tycho Sikkenk[1], Lars Fritz[1], Kris Coester[2], and Kai Schmidt[2] — [1]Universiteit

Utrecht, Institute for Theoretical Physics, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands — [2]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I, Otto-Hahn-Str. 4, D-44221, Dortmund, Deutschland

Geometrical frustration in spin systems often results in a large number of degenerate ground states. In this work we study the antiferromagnetic Ising model on the swedenborgite lattice, a three-dimensional stacking of kagome and triangular layers. The model contains two exchange couplings, one within the kagome layer, another one in between kagome and triangular layers. We investigate the T=0 behaviour of the model in a transverse magnetic field and find a rich phase diagram with both degenerate and non-degenerate phases. Remarkably, for large ratios of out-of-plane coupling over field strength the problem reduces from a three-dimensional quantum model to a two-dimensional classical model at zero temperature.

TT 50.15 Wed 19:00 H18

1/d expansion for the transverse-field Ising model — •Darshan G. Joshi and Matthias Vojta — Institut für Theoretische Physik, Technische Universität Dresden

Analytic 1/d expansion method, previously developed for coupled-dimer magnets, is applied to the transverse-field Ising model (d>1) at zero temperature. We introduce auxiliary Bosons to map the spin Hamiltonian onto a Bosonic Hamiltonian. The hard-core constraint from the physical Hilbert space is implemented using the projection operator. The 1/d expansion is employed in both, the paramagnetic as well as the ferromagnetic, phases. We present 1/d expansion for static as well as dynamic observables, including the phase boundary. We thus have a consistent description of the entire phase diagram, including the quantum critical point.

TT 51: Superconductivity: Tunneling, Josephson Junctions, SQUIDs

Time: Wednesday 15:00–19:00 Location: H19

TT 51.1 Wed 15:00 H19

Investigation of niobium structures for micro-SQUIDs — •Sandra Gottwals[1], Frank Heyroth[2], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, MLU Halle-Wittenberg, Germany

In the presence of the Spin-Nernst-Effect a temperature gradient generates spin accumulations in a metal film. The magnetic moment of these accumulations causes a magnetic field. We intend to measure these low magnetic fields using Nb-based micro-SQUIDs. Superconducting Niobium layers are deposited by e-beam evaporation and protected by capping layers either from Ru or Si. The Niobium layers are patterned by e-beam lithography. We have fabricated test stripes with different width varying from 1000 nm to 20 nm. We will present structural and electrical characterization of Nb stripes patterned by different etching processes. Most of the structures show Ohmic behavior at room temperature. At low temperature a transition to the superconducting state is observed with a transition temperature depending on layer thickness and structures size.

TT 51.2 Wed 15:15 H19

Microwave resonators with high kinetic inductance made from superconducting AlO_x — •Sebastian T. Skacel[1], Micha Wildermuth[1], Julian Münzberg[1], Jan N. Voss[1], Marco Pfirrmann[1], Lucas Radtke[1], Sebastian Probst[1], Martin Weides[1,2], Hannes Rotzinger[1], and Alexey V. Ustinov[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, D-76131 Karlsruhe, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, D-55128 Mainz, Germany

We present superconducting resonators made out of AlO_x with a kinetic inductance fraction - the ratio between kinetic and total inductance of the resonator - close to unity and high quality factors. We show measurements of coplanar waveguide resonators with ultra high impedances and therefore allowing for compact design in the microwave regime. For instance, a coplanar $\lambda/4$ type resonator with resonance frequency of about 5 GHz can be reduced to a length of 180 μm. The resonator impedance depends on the geometry, i.e. length and the width of the central conductor, and its missmatch factor with the 50 Ω feedline changes from about 5 to 30. This also influences the resonator quality factor, due to the altered coupling.
The resonators are fabricated in a simple single layer process starting with the sputter deposited aluminium oxide (AlO_x) on a silicon substrate, followed by optical lithography and reactive ion etch process.

TT 51.3 Wed 15:30 H19

Development of Nb nanoSQUIDs based on SNS junctions for operation in high magnetic fields — •Viacheslav Morosh[1], Benedikt Müller[2], Maria Jose Martinez-Perez[2], Oliver Kieler[1], Thomas Weimann[1], Alexander Zorin[1], Reinhold Kleiner[2], and Dieter Kölle[2] — [1]Physikalisch - Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig — [2]Physikalisches Institut and Center for Quantum Science in LISA$^+$, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen

Investigation of the magnetization reversal of single magnetic nanoparticles requires SQUIDs with high spatial resolution, high spin sensitivity (a few Bohr magneton μ_B) and at the same time sufficient stability in high magnetic fields. We fabricated dc nanoSQUIDs comprising overdamped SNS sandwich-type (Nb/HfTi/Nb) Josephson junctions using optimized technology based on combination of electron beam lithography and chemical-mechanical polishing. Our nanoSQUIDs have Josephson junctions with lateral dimensions $\leq$ 150 nm × 150 nm, effective loop areas $<$ 0.05 μm^2 and the distance between the Josephson junctions $\leq$ 100 nm. The feeding strip lines of the width $\leq$ 200 nm have been realized. The nanoSQUIDs have shown stable operation in external magnetic fields at least up to 250 mT. Sufficiently low level of flux noise resulting in spin sensitivity of few tens $\mu_B/\mathrm{Hz}^{1/2}$ has been demonstrated. A further reduction of the nanoSQUID size using our technology is possible.

This work was supported by the Deutsche Forschungsgemeinschaft (DFG).

TT 51.4 Wed 15:45 H19

Ultra low field magnetic resonance imaging for the investigation of hyperpolarized contrast agents — •M. Rudolph[1], T. Misztal[2], P. Antkowiak[1], H. Meyer[2], R. Kleiner[1], D. Koelle[1], K. Scheffler[3], and K. Buckenmaier[3] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [2]Institut für Anorganische Chemie, Universität Tübingen, Auf der Morgenstelle 18, 72076 Tübingen, Germany — [3]High-Field Magnetic Resonance Center, Max Planck Institute for Biological Cybernetics, Spemannstraße 41, 72076 Tübingen, Germany

In NMR/MRI experiments at ultra low magnetic fields hyperpolarization techniques based on parahydrogen (pH_2) could offer a simple way to circumvent the lack of the low equilibrium polarization of the sample. A chemical exchange reaction, taking place at B_0 fields in the mT range, transfers polarized spins from pH_2 via a transfer catalyst to the sample. This transfer reaction can enhance the sample polarization in B_0 fields in the mT range by a factor of 10^5, offering sample polarizations comparable to polarization fields of 10^3-10^4 T. To investigate these newly developed techniques a SQUID based NMR/MRI system operating at a static magnetic field in the mT range is being developed. By using a SQUID for detecting the NMR Signal, the system can benefit from its very low intrinsic noise level. Additionally, SQUIDs are wide band detectors and can detect the signal of multiple kernels simultaneously. A design of an ultra low field MRI system and first results will be presented.

TT 51.5 Wed 16:00 H19

Sub-gap conductivity of disordered superconducting TaN and NbN thin films — •Marc Scheffler[1], M. Maximilian Felger[1], Moritz Scholze[1], Uwe S. Pracht[1], Martin Dressel[1], Konstantin S. Ilin[2], Michael Siegel[2], and Lara Benfatto[3] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Institut für Mikro- und Nanoelektronische Systeme, KIT — [3]ISC-CNR and Department of Physics, Sapienza University of Rome

Optical spectroscopy studies provide valuable insight into the characteristics of superconductors, such as the superconducting energy gap

and the electrodynamical response of the superfluid condensate and the quasiparticles. Recently, the sub-gap optical conductivity of strongly disordered superconductors has gained substantial attention because of the possibility to observe collective modes that go beyond the classical, BCS-based predictions for the optical properties of superconductors.

We have performed broadband microwave spectroscopy on thin films of NbN (thickness between 3 nm and 20 nm; T_c between 5 K and 13 K) and TaN (thickness 5 nm; T_c around 9 K). The covered temperatures are down to 1.1 K and the frequency range goes up to 50 GHz (which is well below the energy gap). We analyze the real and imaginary parts of the frequency-dependent microwave conductivity and determine the contributions of quasiparticles and Cooper pairs, respectively. We compare these data to Mattis-Bardeen expectations and we discuss them in the light of the ongoing discussion of collective modes in superconductors.

TT 51.6 Wed 16:15 H19

Observation of thermoelectric currents in high-field superconductor-ferromagnet tunnel junctions — •Stefan Kolenda, Michael J. Wolf, and Detlef Beckmann — Institut für Nanotechnologie, Karlsruher Institut für Technologie

We report on the experimental observation of thermoelectric currents in superconductor-ferromagnet tunnel junctions in high magnetic fields [1]. The thermoelectric signals are due to a spin-dependent lifting of particle-hole symmetry, and are found to be in excellent agreement with recent theoretical predictions [2]. The maximum Seebeck coefficient inferred from the data is about -100 μV/K, much larger than commonly found in metalic structures. Our results directly give proof of the coupling of spin and heat transport in high-field superconductors.

[1] S.Kolenda *et al.*, arXiv:1509.05568
[2] A.Ozaeta *et al.*, PRL **112**, 057001 (2014)

TT 51.7 Wed 16:30 H19

"Isolation" of the proximity-induced triplet pairing channel in the superconductor/ferromagnet spin valve — •Pavel Leksin[1,2], Nadir Garifyanov[2], Andrey Kamashev[2], Aidar Validov[2], Yakov Fominov[3,4], Joachim Schumann[1], Vladislav Kataev[1], Jürgen Thomas[1], Bernd Büchner[1,5], and Ilgiz Garifullin[2] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 Dresden, Germany — [2]Zavoisky Physical-Technical Institute, Russian Academy of Sciences, 420029 Kazan, Russia — [3]L. D. Landau Institute for Theoretical Physics, Russian Academy of Sciences, 142432 Chernogolovka, Russia — [4]Moscow Institute of Physics and Technology, 141700 Dolgoprudny, Russia — [5]Institute for Solid State Physics, Technical University Dresden, D-01062 Dresden, Germany

We have studied the proximity induced superconducting triplet pairing in CoO_x/Py1/Cu/Py2/Cu/Pb spin-valve structure. By optimizing the parameters of structures we found a full switching between the normal and superconducting states. To observe an "isolated" triplet spin-valve effect we exploited the oscillatory feature of the magnitude of the ordinary spin-valve effect ΔT_c in the dependence of the Py2-layer thickness d_{Py2}. We determined the value of d_{Py2} at which ΔT_c caused by the ordinary spin-valve effect (the difference in T_c between antiparallel and parallel mutual orientation of magnetizations of the Py1 and Py2 layers) is suppressed. For such a sample a "pure" triplet spin-valve effect which causes the minimum in T_c at the orthogonal configuration of magnetizations has been observed.

15 min. break

TT 51.8 Wed 17:00 H19

Coherent emission of terahertz radiation from intrinsic Josephson junctions in $Bi_2Sr_2CaCu_2O_8$ — •Fabian Rudau[1], Raphael Wieland[1], Xianjing Zhou[2,3], Min Ji[2,3], Nickolay Kinev[4], Luyao Hao[2,3], Ya Huang[2,3], Jun Li[2], Peiheng Wu[2], Takeshi Hatano[3], Valery Koshelets[4], Huabing Wang[2,3], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Germany — [2]Research Institute of Superconductor Electronics, Nanjing University, China — [3]National Institute for Materials Science, Tsukuba, Japan — [4]Kotel'nikov Institute of Radio Engineering and Electronics, Moscow, Russia

Stacks of intrinsic Josephson junctions, made of the high-T_c superconductor $Bi_2Sr_2CaCu_2O_8$, can be used as emitters of electromagnetic waves at terahertz frequencies. Coherent emission from 0.3 to 2.4 THz was detected from large, rectangular or disc-shaped mesa structures. Having a linewidth of only a few MHz, emission powers of several tens of microwatt can be produced for single stacks and up to 0.61 mW for an array of mesas.

Since the mechanisms of synchronizing all the junctions in the stack is still not fully understood, we investigated the temperature distribution and electromagnetic standing waves in such stacks, as well as the generation of terahertz radiation, using a combination of electric transport measurements, direct radiation detection and low temperature scanning laser microscopy. Recent experimental results from our collaboration will be presented and compared to numerical simulations.

TT 51.9 Wed 17:15 H19

Stabilized superconductivity in periodically driven Josephson junction chains — •Junichi Okamoto[1,2,3], Andrea Cavalleri[4,5], and Ludwig Mathey[1,2,3] — [1]Center for Optical Quantum Technologies, University of Hamburg, Hamburg, Germany — [2]Institute of Laser Physics, University of Hamburg, Hamburg, Germany — [3]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany — [4]Max Planck Institute for the Structure and Dynamics of Matter — [5]University of Oxford

Motivated by recent pump-probe experiments indicating enhanced coherent c-axis transport in an underdoped YBCO, a typical high-T_c superconductor, we study a system of capacitively coupled alternating Josephson junctions periodically driven by laser pulses. Using Langevin simulations, we show that the reduction of current fluctuations is realized through the Kapitza effect for high-frequency driving. In this regime superfluid density calculated from the imaginary part of conductivity is indeed enhanced compared to the thermal value. Calculations based on effective models with renormalized parameters explain this enhancement of superfluid density and other features of driven states.

TT 51.10 Wed 17:30 H19

Self-heating in Josephson junction chains: new insight from old circuits — •Jared Cole[1], Michael Marthaler[2], and Timothy Duty[3] — [1]Chemical and Quantum Physics, School of Applied Sciences, RMIT University, Melbourne, Victoria 3001, Australia — [2]Institute für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]Centre for Engineered Quantum Systems (EQuS), School of Physics, University of New South Wales, Sydney, New South Wales 2052, Australia

The conduction properties of arrays of Josephson junctions are been studied for decades, yet the experimental results never really match the predictions of the idealised theoretical models. Many reasons have been given for this, including imperfections in the measurement, in the fabrication process or in the theoretical models used. Recently, using a combination of systematic numerical and experimental studies, the gap between theory and experiment is closing. As an example of this, we discuss the role of self-heating in the transport properties of one-dimensional Josephson junction chains. We show tantalising experimental measurements and how these can be compared to various theoretical models for the self-heating processes within the chains.

TT 51.11 Wed 17:45 H19

Quasicharge depinning in bilinear Josephson juncton arrays — •Samuel Wilkinson, Nicolas Vogt, and Jared Cole — Chemical and Quantum Physics, School of Applied Sciences, RMIT University, Melbourne 3001, Australia

Bilinear Josephson junction arrays have been the subject of experimental studies, where interesting threshold, Coulomb drag and current mirror behaviour have been observed. Theoretically, the precise mechanisms are not currently well understood. We have applied the theory of quasicharge depinning, which has previously been successfully in describing linear arrays. Here we present the results of numerical simulations which offer insight into some of the experimentally observed phenomena, and suggests possible new effects which may be observed at high voltages.

15 min. break

TT 51.12 Wed 18:15 H19

Antibunched photons from inelastic Cooper-pair tunneling — •Juha Leppäkangas[1,2], Mikael Fogelström[1], Alexander Grimm[3], Max Hofheinz[3], Michael Marthaler[2], and Göran

Johansson[1] — [1]Microtechnology and Nanoscience, MC2, Chalmers University of Technology, Göteborg, Sweden — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Université Grenoble Alpes, INAC-SPSMS, Grenoble, France

We demonstrate theoretically that charge transport across a Josephson junction, voltage-biased through a resistive environment, produces antibunched photons. We develop a continuous-mode description of the emitted radiation field in a semi-infinite transmission line terminated by the Josephson junction. Within a perturbative treatment in powers of the tunneling coupling across the Josephson junction, we capture effects originating in charging dynamics of consecutively tunneling Cooper pairs. We find that within a feasible experimental setup the Coulomb blockade provided by high zero-frequency impedance can be used to create antibunched photons at a very high rate and in a very versatile frequency window ranging from a few GHz to a THz.

TT 51.13 Wed 18:30 H19

Josephson switching current investigated in a scanning tunneling microscope junction — •Jacob Senkpiel[1], Berthold Jäck[1], Matthias Eltschka[1], Markus Etzkorn[1], Christian R. Ast[1], and Klaus Kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart — [2]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Employing the $I(V)$-characteristics of a scanning tunneling microscope (STM) Josephson junction to directly determine the local order parameter of a superconductor would give a powerful tool to understand superconductivity on the atomic scale. Recent research in this field led to some valuable insights to this technique [1,2]. Being able to perform not only voltage but also current biased measurements of the same junction gives us a new approach to study the physics involved in the Josephson effect. Interestingly a comparison of the current and the voltage biased measurements shows that the Josephson switching current corresponds to the current value of the maximum in the voltage biased measurement. In contrast to conventional planar tunneling geometries, an STM allows for precise control of the tunneling resistance and makes it possible to tune the Josephson coupling energy. Using this ability we find, that the switching current is proportional to the square of the Josephson coupling energy.
[1] B. Jäck et al., APL **106**, 062904 (2015)
[2] C.R. Ast et al., arXiv:1510.08449

TT 51.14 Wed 18:45 H19

Cooper pair splitters beyond the Coulomb blockade regime — •Ehud Amitai[1], Rakesh P. Tiwari[1], Stefan Walter[2], Thomas L. Schmidt[3], and Simon E. Nigg[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [2]Institute for Theoretical Physics, University Erlangen Nuernberg, Staudtstrasse 7, 91058 Erlangen, Germany — [3]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg

We consider the setup of a conventional s-wave Cooper pair splitter. However, we consider the charging energies in the quantum dots to be finite and smaller than the superconducting gap. We find analytically that at low energies the superconductor mediates an inter-dot tunneling term, the spin symmetry of which is influenced by a finite Zeeman field. This effect, together with an electrical tuning scheme of the quantum dot levels, can be used to engineer a non local triplet state on the two quantum dots, thereby extending the non-local state engineering capabilities of the Cooper pair splitter system.

TT 52: Focus Session: Realistic Dynamical Mean-Field Approaches to Correlated Quantum Materials

Theoretical investigations of the properties of correlated quantum materials require not only the application of electronic structure theories but also of many-body techniques. Here realistic dynamical mean-field approaches have proved to be a conceptual breakthrough, leading to important new insights into the physics of electronically correlated materials. This is a very active field of research, which will be reviewed by internationally acknowledged experts.

Organizers: Roser Valenti (Goethe-Universität Frankfurt am Main)
and Dieter Vollhardt (Universität Augsburg)

Time: Wednesday 15:00–18:15 Location: H20

Invited Talk TT 52.1 Wed 15:00 H20

Hund's Metals: a New Road to Strongly Correlated Electron Behavior — •Gabriel Kotliar — Rutgers University Piscataway NJ USA

Over the past thirty years, substantial effort has been devoted to describing materials near a Mott transition. In these systems, correlation effects (i.e. departures from free electron behavior) arise from strong on site repulsion (Hubbard U terms). Prototypical materials are V_2O_3. Recently attention has turned to a different origin of strong correlation phenomena which is rooted in the Hund's coupling J term, starting with LDA+DMFT studies in the iron based high temperature superconductors and the ruthenium oxides. We will argue that Hund's metals are well described by Dynamical Mean Field Theory, and are characterized by the phenomena of orbital spin separation[2,3]. We will present an elementary introduction to the theory of Hund's metals stressing the experimental signatures which distinguishes them from materials near a Mott transition
[1] K. Haule and G. Kotliar, New J. Phys. **11**, 025021 (2009).
[2] C. Aron and G. Kotliar, PRB **91**, 041110 (2015).
[3] K. Stadler et. al., PRL **115**, 136401 (2015)

Invited Talk TT 52.2 Wed 15:30 H20

Screened Exchange Dynamical Mean Field Theory — •Silke Biermann — Centre de Physique Theorique, Ecole Polytechnique, Palaiseau, France

Dynamical mean field theory (DMFT), in conjunction with electronic structure techniques has led to tremendous progress in the description of excited state properties of materials with strong electronic Coulomb correlations. One of the main challenges nowadays consists in refining the interface of electronic structure and many-body theory in order to develop quantitatively accurate predictive schemes. We review recent efforts of incorporating dynamical screening effects into a DMFT-based description of correlated materials [1]. Such effects can stem either from higher energy degrees of freedom that have been integrated out [2] or from nonlocal processes that are effectively backfolded into a local description. This can be conveniently done by combined many-body perturbation theory and dynamical mean field theory ("GW+DMFT") techniques [3]. These insights lead to a simple but efficient scheme, dubbed "Screened exchange dynamical mean field theory" [4], which can be understood as an approximation to GW+DMFT, or as a non-perturbative dynamical generalization of Hedin's Coulomb-hole-screened-exchange approximation. In particular, it includes non-local exchange beyond the local density approximation and dynamical screening beyond standard DMFT techniques.
[1] S. Biermann, JPCM **26**, 173202 (2014)
[2] J. M. Tomczak et al., PRB **90**, 165138 (2014)
[3] T. Ayral et al., PRL **109**, 226401 (2012)
[4] A. van Roekeghem et al., PRL **113**, 266403 (2014);
A. van Roekeghem et al., EPL **108**, 57003 (2014)

Invited Talk TT 52.3 Wed 16:00 H20

Dynamical Screening in Correlated Electron Materials — •Philipp Werner — University of Fribourg, 1700 Fribourg, Switzerland

I will discuss efficient methods for treating dynamically screened interactions within dynamical mean field theory (DMFT). These methods

allow to incorporate ab-initio estimates of the local Coulomb matrix elements into low-energy effective models, and to treat the screening from nonlocal Coulomb interactions within extended DMFT or more sophisticated formalisms. I will present results from applications to simple model systems and strongly correlated materials, and some insights into the real-time dynamics of screening obtained with a recent nonequilibrium implementation of extended DMFT.

15 min. break

Invited Talk TT 52.4 Wed 16:45 H20
Lattice stability of correlated electron materials — •Ivan Leonov — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany

The theoretical understanding of the interplay of electronic correlations and lattice, and, in particular, the realistic description of strongly correlated electron materials, is one of the most challenging problems in condensed matter physics. In this talk, I will report results of the application of the LDA+DMFT computational scheme to explore the electronic and structural properties of correlated materials from first principles. Our results show that electronic correlations are crucial to explain the electronic state, equilibrium crystal structure, and lattice stability of correlated materials [1]. In addition, I discuss application of the LDA+DMFT approach to compute the interatomic forces, which makes it possible to determine the atomic displacements and to perform structural optimization of correlated materials [2].

[1] I. Leonov *et al.*, PRL **106**, 106405 (2011);
I. Leonov *et al.*, PRL **115**, 106402 (2015);
I. Leonov *et al.*, PRB **91**, 195115 (2015)
[2] I. Leonov *et al.*, PRL **112**, 146401 (2014)

Invited Talk TT 52.5 Wed 17:15 H20
Tin Foil at the Nanometer Scale - from Electronic Correlations to Topological Physics — •Ralph Claessen — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, 97074 Würzburg, Germany

With respect to its electronic properties and compared to its semiconducting siblings C, Si, and Ge the group IV element tin (Sn) has always been a somewhat profane material. At ambient conditions Sn is a white-silverish metal (tetragonal β-Sn) and as tin foil has long been used for wrapping food (nowadays replaced by aluminum foil). At 13.2° C a structural phase transition into the diamond-like α-phase occurs, known as "tin pest" which in former times posed a severe threat to church organ pipes in the winter time.

I will report on recent studies of (ultra)thin Sn films in which this elemental material displays highly interesting topological physics and correlation effects, otherwise seen only in materials of much higher structural or chemical complexity. This includes (1) the realization of compressively strained α-Sn as 3D topological insulator (TI), (2) our attempts to grow the Sn analogue of graphene, so-called stanene, which is predicted to be a 2D TI, and (3) the formation of triangular Sn lattices on semiconductor substrates, which display Mott-Hubbard physics and even magnetic instabilities despite the frustrated geometry.

Invited Talk TT 52.6 Wed 17:45 H20
Electron Correlations in Nanosystems and 2D Materials: What's so Different from Bulk? — •Tim Wehling — University of Bremen, Bremen, Germany

To date, experimental nanofabrication techniques offer atomic scale control of correlated electron materials from Mott insulators and magnets to superconductors. Here, we discuss correlation effects in atomic scale structured systems based on a combination of first-principles and many-electron techniques. We show that substrate, environmental and doping effects can change Coulomb interactions in monolayer thin 2d materials on the eV scale [1], which has strong influence on electronic excitations and collective modes [2]. With two sets of magnetic systems, a Cr (001) surface and hydrogenated Fe adatoms on Pt (111), we address then how electronic hybridization and kinetic terms can be manipulated at the atomic scale. These terms control in both systems a delicate interplay of charge, spin, and orbital degrees of freedom and allow us to turn electronic correlation phenomena like the Kondo effect on and off [3].

[1] M. Rösner et al., PRB **92**, 085102 (2015)
[2] A. Steinhoff et al., Nano Lett. **14**, 3743 (2014)
[3] A. Khajetoorians et al, Nature Nanotech. **10**, 958 (2015).

TT 53: Low-Dimensional Systems: 1D - Theory

Time: Wednesday 15:00–18:15 Location: H21

TT 53.1 Wed 15:00 H21
Topological phases and phase transitions of interacting fermions in 1D — •Ruben Verresen — MPI-PKS, Dresden, Germany

Not all phases of matter can be described by local order parameters. One such unconventional class is that of Symmetry Protected Topological (SPT) phases, where the presence of a symmetry and a gap ensures interesting topological effects. Topological insulators are a prominent example, but the landscape of SPTs becomes more interesting when we allow for interactions. Here we focus on 1D fermionic systems. In 2010 it was discovered that if the Hamiltonian conserves fermionic parity and is time reversal invariant, there are exactly eight gapped phases– one being the celebrated Kitaev chain with Majorana edge modes. This analysis led to a general classification of SPT phases. We revisit these unconventional 1D fermionic phases in concrete models, both to discuss the conceptual underpinning of SPTs and to characterize the critical theories when tuning between these eight phases. The latter is of particular interest since the understanding of phase transitions between SPTs is still a very young field.

TT 53.2 Wed 15:15 H21
Dynamics of photo excitations in 1D-Hubbard systems — •Thomas Köhler and Salvatore R. Manmana — Institut für Theoretische Physik, Universität Göttingen, Germany

We compute the dynamics following a photo excitation in one dimensional Hubbard systems at different temperatures T using matrix product state (MPS) approaches. We discuss the effect of temperature on the propagation of these excitations and give an outlook for systems with time dependent Hamiltonians.

Financial support via DFG through CRC 1073 "Atomic scale control of energy conversion", project B03 is gratefully acknowledged.

TT 53.3 Wed 15:30 H21
Finite-temperature dynamics of Spin-1 Heisenberg chains via Matrix Product States — Thomas Köhler[1], Alexander Tiegel[1], •Salvatore R. Manmana[1], and Andreas Honecker[2] — [1]Institut für Theoretische Physik, Universität Göttingen, 37077 Göttingen — [2]LPTM, Université de Cergy-Pontoise, France

The S=1 Heisenberg chain is an archetypal model of quantum magnetism that realizes a 1D symmetry protected topological (SPT) insulator which is adiabatically connected to the AKLT state. Here, we investigate in detail the temperature dependence of dynamical spectral functions for S=1 Heisenberg chains using finite-temperature Matrix Product State (MPS) approaches. By applying open boundary conditions (OBC), we are able to investigate for signatures of the edge states and their evolution upon increasing the temperature.

Financial support via DFG through CRC 1073 "Atomic scale control of energy conversion", project B03, and by the Helmholtz Virtual Institute "New States of Matter and their Excitations", project P6, is gratefully acknowledged.

TT 53.4 Wed 15:45 H21
Quantum Monte Carlo studies of the spin dynamics in the spin-1 Heisenberg chain — •Jonas Becker and Stefan Wessel — Institut für Theoretische Festkörperphysik, JARA-FIT and JARA-HPC, RWTH Aachen University, 52056 Aachen, Germany

The dynamic spin structure factor $S(k, \omega)$ of the antiferromagnetic isotropic spin $S = 1$ Heisenberg chain is studied at finite temperature. Quantum Monte Carlo simulations with the stochastic series expansion scheme are performed to extract this dynamic observable for individual Matsubara frequencies. Then a stochastic analytic continuation method is applied to extract the real-frequency spin structure factor from the imaginary frequency data. Simulations for low temper-

atures are performed with high accuracy and the results are compared to DMRG data [1]. We also focus on the spectrum's multi-magnon continuum and show that performing the analytic continuation in the over-fitting regime produces additional features therein. Finally, the temperature dependence of the dynamic spin structure factor $S(k, \omega)$ is presented.

[1] S. White and I. Affleck. PRB **77**, 134437 (2008)

TT 53.5 Wed 16:00 H21

ESR modes in a Strong-Leg Ladder in the Tomonaga-Luttinger Liquid Phase — •S. Zvyagin[1], M. Ozerov[2], M. Maksymenko[3], J. Wosnitza[1], A. Honecker[4], C.P. Landee[5], M. Turnbull[5], S. Furuya[6], and T. Giamarchi[6] — [1]HLD-HZDR, Dresden, Germany — [2]Radboud University, Nijmegen, The Netherlands — [3]Weizmann Institute of Science, Rehovot, Israel — [4]Universite de Cergy-Pontoise, Cergy-Pontoise Cedex, France — [5]Clark University, Worcester, MA, USA — [6]University of Geneva, Geneva, Switzerland

Magnetic excitations in the strong-leg quantum spin ladder compound $(C_7H_{10}N)_2CuBr_4$ (known as DIMPY) in the field-induced Tomonaga-Luttinger spin liquid phase are studied by means of high-field electron spin resonance (ESR) spectroscopy. The presence of a gapped ESR mode with unusual non-linear frequency-field dependence is revealed experimentally. Using a combination of analytic and exact diagonalization methods, we compute the dynamical structure factor and identify this mode with longitudinal excitations in the antisymmetric channel. We argue that these excitations constitute a fingerprint of the spin dynamics in a strong-leg spin-1/2 Heisenberg antiferromagnetic ladder and owe its ESR observability to the uniform Dzyaloshinskii-Moriya interaction.

This work was partially supported by the DFG and Helmholtz Gemeinschaft (Germany), Swiss SNF under Division II, and ERC synergy UQUAM project. We acknowledge the support of the HLD at HZDR, member of the European Magnetic Field Laboratory (EMFL).

TT 53.6 Wed 16:15 H21

Tomonaga-Luttinger to Luther-Emery crossover in spin-gapped metals — Jonas Greitemann[1,3], Stephan Hesselmann[1], Stefan Wessel[1], Fakher Assaad[2], and •Martin Hohenadler[2] — [1]RWTH Aachen, Germany — [2]University of Würzburg, Germany — [3]LMU Munich, Germany

We consider the crossover between the gapless Tomonaga-Luttinger and the spin-gapped Luther-Emery fixed point as a function of distance in models with attractive backscattering. Our quantum Monte Carlo results for extended Hubbard and Holstein models reveal the impact of this crossover on correlation functions, Luttinger parameters, and critical values for the charge-density-wave transition. The implications for our understanding of the Holstein-Hubbard model are discussed.

15 min. break

TT 53.7 Wed 16:45 H21

Effective few-leg ladder models for correlated wires on substrates — •Anas Abdelwahab[1], Eric Jeckelmann[1], and Martin Hohenadler[2] — [1]Leibniz Universität Hannover, Germany — [2]Universität Würzburg, Germany

Correlated quantum wires deposited on a substrate constitutes a challenge for existing analytical and numerical methods. We develop a mapping onto 2D ladder models based on the Lanczos algorithm. Possibilities and limitations of truncating the 2D ladder onto effective few-leg ladder models are discussed. We use DMRG and quantum Monte Carlo methods to investigate if an effective few-leg ladder model is a good approximation for a correlated wire on substrate. We perform a comparison with a two-leg effective model [1] and discuss the modeling of Luttinger liquids on semiconducting substrates.

Support from the DFG through the Research Units FOR 1700 and FOR 1807 is gratefully acknowledged.

[1] A. Abdelwahab, E. Jeckelmann, and M. Hohenadler, PRB **91**, 155119 (2015)

TT 53.8 Wed 17:00 H21

Thermodynamic and spectral properties of one-dimensional electron-phonon models in the adiabatic limit — •Manuel Weber, Fakher F. Assaad, and Martin Hohenadler — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

In one-dimensional electronic systems at half-filling, electron-phonon coupling can lead to lattice dimerization accompanied by charge-density or bond-density wave order. According to Peierls' theorem, the ground state is ordered for any nonzero coupling when quantum lattice fluctuations are neglected. In this adiabatic limit, the lattice displacements become classical variables that can be sampled in a Monte Carlo simulation. For each phonon configuration, the resulting fermionic Hamiltonian can be diagonalized exactly. Considering the Holstein model and the Su-Schrieffer-Heeger model, we study the formation of the Peierls-insulating ground state as a function of temperature. At low temperatures, we observe a peak in the specific heat associated with the opening of a band gap, and the formation of shadow bands as well as polaron signatures in the single-particle spectrum.

TT 53.9 Wed 17:15 H21

Thermodynamics, contact and density profiles of the repulsive Gaudin-Yang model — •Andreas Klümper[1] and Ovidiu Patu[2] — [1]Universität Wuppertal, Gauss-Strasse 20, 42119 Wuppertal — [2]Institute for Space Sciences, Bucharest-Magurele, R 077125

We address the problem of computing the thermodynamic properties of the repulsive one-dimensional two-component Fermi gas with contact interaction (Gaudin-Yang model). We derive an exact system of only two non-linear integral equations for the thermodynamics of the homogeneous model. This system allows for an easy and extremely accurate calculation of thermodynamic properties circumventing the difficulties associated with the truncation of the thermodynamic Bethe ansatz system of equations. We present extensive results for the densities, polarization, magnetic susceptibility, specific heat, interaction energy, Tan contact and local correlation function of opposite spins. Our results show that at low and intermediate temperatures the experimentally accessible contact is a non-monotonic function of the coupling strength. As a function of the temperature the contact presents a pronounced local minimum in the Tonks-Girardeau regime which signals an abrupt change of the momentum distribution in a small interval of temperature. The density profiles of the system in the presence of a harmonic trapping potential are computed using the exact solution of the homogeneous model coupled with the local density approximation. At finite temperature the density profile presents a double shell structure (partially polarized centre and fully polarized wings) only when the polarization in the center of the trap is above a critical value.

TT 53.10 Wed 17:30 H21

Properties of the single-site reduced density matrix in the Bose-Bose resonance model in equilibrium and in quantum quenches — •Florian Dorfner and Fabian Heidrich-Meisner — Ludwig-Maximilians-Universität München, Germany

We study properties of the single-site reduced density matrix in the Bose-Bose resonance model as a function of system parameters. This model describes a single-component Bose gas with a resonant coupling to a molecular state, here defined on a lattice. We study the eigenstates of the single-site reduced density matrix in the various quantum phases of this system. Since the Hamiltonian conserves only the global particle number but not the number of bosons and molecules individually, these eigenstates, referred to as optimal modes, can be nontrivial linear combinations of bare eigenstates of the molecular and boson particle number. We numerically analyze the optimal modes and their weights, the latter giving the importance of the corresponding state, in the ground state of the Bose-Bose resonance model and find that the single-site von Neumann entropy is sensitive to the position of the phase boundaries. We explain the structure of the optimal modes and their weight spectra using perturbation theory and via a comparison to results for the one-species Bose-Hubbard model. Further, we study the dynamical evolution of the optimal modes and of the single-site entanglement entropy in two quantum quenches that cross phase boundaries between different phases of the model. For our numerical calculations, we use exact diagonalization and the density matrix renormalization group method.

TT 53.11 Wed 17:45 H21

Fractional Wigner oscillations in two-dimensional topological insulators — •Niccolo Traverso Ziani[1], Francois Crépin[2], and Bjoern Trauzettel[1,3] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [2]Laboratoire de Physique Théorique de la Matière Condensée, UPMC, CNRS UMR 7600, Sorbonne Universités, 4 place Jussieu, 75252 Paris Cedex 05, France — [3]Department of Physics, University of California, Berkeley, California 94720, USA

In finite electronic systems, when electron-electron interactions dominate over kinetic energy, electrons tend to form regular lattices, called Wigner molecules. One dimensional electrons do not represent an exception [1]. Importantly, for strong interactions, the Wigner molecule becomes an almost classical state and any dependence on the spin degree of freedom is lost. This behaviour is antithetical to the concept of spin-momentum locking characterizing the helical edges of two-dimensional topological insulators (helical Luttinger liquids) [2]. The compromise between strong interactions and spin-momentum locking leads, in helical systems, to a Wigner oscillation of fermions with fractional charge e/2 [3]. This fractional oscillation is also characterized by strongly anisotropic spin-spin correlations.

[1] I. Safi and H. J. Shulz, PRB **59**, 3040 (1999)
[2] C. Wu, B., A. Bernevig, S.-C. Zhang, PRL **96**, 105401 (2006)
[3] N. Traverso Ziani, F. Crépin, B. Trauzettel, PRL **115**, 206402 (2015).

TT 53.12 Wed 18:00 H21

Time-dependence of Spin-Orbital Excitations in the one dimensional Kugel-Khomskii model — •Mirco Marahrens and Maria Daghofer — Institut für Funktionelle Materie und Quantentechnologien, University of Stuttgart, Stuttgart, Baden-Wuerttemberg, Germany

Using the technique of time-dependent Density Matrix Renormalization Group (tDMRG) we investigating the behaviour of spin and orbital dynamics in the Kugel-Khomskii model. The model couples an SU(2) algebra for the spin with and orbital degree of freedom, where a crystal field breaks SU(2) symmetry. For the case of an orbital splitting larger than the magnetic coupling, the ground state has antiferromagnetic (AFM) and ferro-orbital (FO) order. Initial states are prepared as deviations from this order, as might arise through a temporary quench of crystal field. An example that will be analyzed is the spin-orbit separated propagation of fractionalized elementary excitations [1]. We discuss ongoing work on this issue and the different aspects of the results obtained so far.

[1] J. Schlappa et al., Nature **485**, 82 (2012)

TT 54: Transport: Carbon Nanotubes

Time: Wednesday 15:00–18:15 Location: H22

TT 54.1 Wed 15:00 H22

Carbon nanotubes in high magnetic field — •Magdalena Marganska[1], Peter L. Stiller[2], Alois Dirnaichner[2], Daniel R. Schmid[2], Michael Niklas[1], Andreas K. Hüttel[2], Christoph Strunk[2], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

A parallel magnetic field affects strongly the electronic transport through a carbon nanotube (CNT) via its coupling to the orbital degree of freedom. Although such a wire-like system can host neither the fully developed Hofstadter butterflies nor Landau levels, the magnetic field has nevertheless a deep influence on the CNT's spectrum and wave functions. We report here on the results of both theoretical calculations and experimental measurements of a CNT quantum dot. The two experimental results on which we focus are a strong suppression of the conductance by the parallel magnetic field and an unusual evolution of the spectral lines. The unique boundary conditions, which couple the transverse and longitudinal momentum, are responsible both for decreased transmission through the CNT and for the remarkable dependence of the longitudinal momentum on the magnetic field.

TT 54.2 Wed 15:15 H22

Co-sputtered Mo/Re superconducting coplanar resonators compatible with carbon nanotube growth — •Stefan Blien, Peter L. Stiller, Karl Götz, Ondrej Vavra, Thomas Huber, Thomas Mayer, Christoph Strunk, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Carbon nanotubes are simultaneously prototypical single electron tunneling devices and nano-electromechanical resonators. In particular for "ultraclean" devices, where the nanotube is grown in a last fabrication step over pre-existing chip structures, highly regular quantum spectra and high mechanical quality factors emerge. Targeting optomechanical experiments, a coupling of these devices to on-chip superconducting coplanar waveguide resonators is highly desirable. The conditions for in-situ growth of carbon nanotubes over metal contacts are quite detrimental to most superconductors: the CVD growth process takes place in a hydrogen/methane atmosphere heated up to 900°C. We present data on transmission line resonators fabricated of a co-sputtered molybdenum rhenium alloy that withstand CVD and remain superconducting with critical temperatures up to 8K after growth. Resonant operation at cryogenic temperatures is demonstrated, and the behaviour is highly consistent with a combination of Mattis-Bardeen theory and two-level systems in the substrate.

TT 54.3 Wed 15:30 H22

Franck-Condon physics in a few-electron 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

Franck-Condon sidebands in the transport spectroscopy of suspended carbon nanotubes provide a beautiful nano-electromechanical model system where quantized harmonic oscillator behaviour becomes visible. We present measurements on a strongly localized few-electron system ($0 \leq N_{\mathrm{el}} \leq 2$), where the coupling of single electron tunneling and vibrational motion arises solely at finite magnetic fields parallel to the carbon nanotube axis. The Franck-Condon parameter g increases with magnetic field and saturates above $B \approx 4$ T. The behaviour of the sidebands dressing the electronic ground and excited quantum state resonances is compared, and tentative models are discussed.

TT 54.4 Wed 15:45 H22

Secondary interference from trigonal warping in clean carbon-nanotubes — Alois Dirnaichner[1,2], •Miriam del Valle[2], Karl Götz[1], Felix Schupp[1], Nicola Paradiso[1], Milena Grifoni[2], Andreas Hüttel[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg — [2]Institute for Theoretical Physics, University of Regensburg

We investigate experimentally and theoretically a Fabry-Perot resonator based on a clean carbon nanotube. The trigonal warping of the Dirac cones away from the charge degeneracy point leads to a superstructure in the interference pattern. This secondary interference results from the presence of the valley degree of freedom. Single wall carbon nanotubes can be classified to be either zigzag, armchair, zigzag-like, or armchair-like. In any armchair case two interferometer channels with different wave vectors exist; specifically in the armchair-like (chiral with finite-$k_{\parallel}$ Dirac point) nanotube case these two channels additionally mix on reflection at the interferometer ends. The wave vector difference depends on the chiral angle; this way we can use the resulting slow modulation of the average conductance to estimate the chiral angle of the measured nanotube. 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.

TT 54.5 Wed 16:00 H22

Emerging Kondo screening and many-body Kramers entanglement in a carbon nanotube — •Michael Niklas[1], Sergey Smirnov[1], Davide Mantelli[1], Magdalena Margańska[1], Jean-Pierre Cleuziou[2], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute Néel, CNRS and Université Grenoble Alpes, BP 166, 38042 Grenoble, France

The entanglement of quantum states is at the heart of the Kondo effect. In its simplest realization, interactions between a localized spin and itinerant electrons give rise to an entangled singlet ground state with no net spin. Carbon nanotubes offer the possibility to study the emergence of this entanglement in a system with orbital and spin degrees of freedom by simply tuning a gate voltage. Here we investigate the magnetospectrum of a carbon nanotube and find the disappearance of some inelastic excitation lines when sweeping the gate voltage

from the weak to the strong coupling regime where Kondo behavior is observed. We consider the global $SU(2) \otimes SU(2)$ symmetry associated to the two Kramers channels of a carbon nanotube and find that only excitations involving flips of the Kramers pseudospins are observed in the Kondo regime, revealing that those pseudospins are fully screened by the conduction electrons.

TT 54.6 Wed 16:15 H22

Mode splitting in zig-zag carbon nanotubes — Jhon González[1], Gilles Buchs[2], •Dario Bercioux[3,4], and Andres Ayuela[1,3] — [1]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, E-20018 Donostia-San Sebastián, Spain — [2]Centre Suisse d'Electronique et de Microtechnique (CSEM) SA, Rue de l'Observatoire 58, CH-2002 Neuchâtel, Switzerland — [3]Donostia International Physics Center (DIPC), E-20018 Donostia-San Se- bastián, Spain — [4]IKERBASQUE, Basque Foundation of Science, E-48011 Bilbao, Spain

We investigate theoretically the electron scattering properties of defected and free-standing zig-zag single-walled carbon nanotubes. The variation of the chemical potential, realized in the suspended region, produces quasi-bound states, which compete with the ones created by multiple defects [1]. We show that a particular configuration of the tube defects produces a degeneracy lifting in the metallic branches of the nanotube. As a consequence we observe a doubling or splitting of the quasi-bound states. We also observe a particle-hole symmetry breaking due to selection rules associated to the interplay of tube and defects [2]. Our predictions are supported by an experimental case where a partially suspended zig-zag tube shows split quasi-bound states between defects induced by Ar^+ ions [1] Our results find applications in angular momentum filtering as well as in THz optics. [3].

[1] D. Bercioux *et al.*, Phys. Rev. B **83**, 165439 (2011).
[2] L. Mayrhofer and D. Bercioux, Phys. Rev. B **84**, 115126 (2011).
[3] J. González *et al.*, *submitted.*

15 min. break

Invited Talk TT 54.7 Wed 16:45 H22

Cooling a nanomechanical resonator by electron transport in hybrid devices. — •Gianluca Rastelli, Pascal Stadler, and Wolfgang Belzig — Universität Konstanz, Germany

A still open challenge in nanoelectromechanical systems is the achievement of active cooling using purely electron transport in devices fabricated with bottom-up techniques as, for instance, carbon nanotube quantum dots suspended between two electric nano-contacts. Owing to the interaction between the electrons and the flexural mechanical modes, the electron transport results inelastic. The vibration assisted tunneling processes give rise to a mechanical damping and, for an applied bias-voltage, to a steady non-equilibrium phonon occupation of the resonator. I will discuss these effects for: (i) spin-polarised current between two ferromagnets [1,2] and (ii) sub-gap Andreev current between a superconductor and normal metal [3]. I will show that ground state cooling of the resonator can be achieved for realistic parameters of the system. I will also discuss the signatures of the non-equilibrium state of the resonator in the current-voltage characteristic.

[1] P. Stadler, W. Belzig, and G. Rastelli, PRL **113**, 047201 (2014).
[2] P. Stadler, W. Belzig, and G. Rastelli, PRB **91**, 085432 (2015).
[3] P. Stadler, W. Belzig, and G. Rastelli, arXiv:1511.04858.

TT 54.8 Wed 17:15 H22

Electronic transport in strained, bent and deformed nanotubes in presence of magnetic field — Magdulin Dwedari[1], Eric Kleinherbers[1], Lennart Korsten[1], Thomas Stegmann[1,2], and •Nikodem Szpak[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [2]Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca

Due to imminent applications in nanoelectronics it is of high interest to better understand the precise conductance properties of various types carbon nanotubes. Since low-energy electronic excitations in graphene behave like massless Dirac fermions the current flow can be approximated semiclassically and used as a guide in the design of conducting nanotube-elements. We compare two alternative approaches to the electronic transport: a) current flows obtained with the non-equillibrium Green's function (NEGF) method from the tight-binding model with local strain and external magnetic field, b) classical trajectories for relativistic point particles moving in a curved surface with pseudo-magnetic and magnetic field. We discuss several setups and effects of special interest: gap engineering in strained nanotubes with parallel magnetic field, magnetic field-effect transistor and current flow paths in bent and deformed nanotubes. We compare results obtained theoretically with numerical simulations.

TT 54.9 Wed 17:30 H22

Electron transport in defective metallic and semiconducting carbon nanotubes — •Fabian Teichert[1,2,4], Andreas Zienert[3], 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

The present work describes the transport properties of metallic and semiconducting CNTs with randomly positioned realistic defects, namely mono- and divacancies. The calculations are based on a fast, linearly scaling recursive Green's function formalism, allowing us to treat large systems quantum-mechanically. The electronic structure is described by a density-functional-based tight-binding model.

In [1], transmission spectra of metallic CNTs with many defects are studied comprehensively with a statistical analysis and diameter-dependent localization lengths are extracted. We extend this work to defect mixtures and show that the total localization length can be reduced to the ones of CNTs with one defect type. Based thereon, we show how to estimate or even predict the conductance of CNTs with an arbitrary number of defects of different types. Finally, we focus on defective semiconducting CNTs and show the influence of the structural parameters – the diameter and the chiral angle – on the conductance and the localization length.

[1] F. Teichert et al., NJP **16** (2014) 123026

TT 54.10 Wed 17:45 H22

Shot noise of excited states in a CNT quantum dot — •Daniel Steininger, Nicola Paradiso, Michael Schafberger, Michael Niklas, Milena Grifoni, and Christoph Strunk — University of Regensburg

Shot noise experiments are a fundamental tool for studying the correlation between carriers in mesoscopic devices. The study of fluctuations provides information that is not accessible by current measurements alone. Here we report on simultaneous measurements of shot noise and conductance of carbon nanotube quantum dots. The high sensitivity of our setup (of the order of 10^{-29} A^2/Hz) allows us to observe the change in the shot noise induced by each CNT excited states. The experimental results are discussed in light of a theory accounting for shot noise effects in the sequential tunnelling limit. In addition we investigate the shot noise in regions of the stability diagram with negative differential conductance.

TT 54.11 Wed 18:00 H22

Electronic Transport through surface functionalized noble metal nanoparticles: Studied at the single object level — •Tuhin Shuvra Basu, Simon Diesch, and Elke Scheer — Fachbereich Physik, Universität Konstanz, Universitätsstraße 10, 78457 Konstanz, Germany

Surface functionalized noble metal nanoparticles exhibit strong plasmonic effects which can be tuned by changing the size of the nanoparticle and by altering the surface functionalization. Additionally due to intraband splitting in ultra-small nanoparticles, they often exhibit weak photoluminescence (PL) [1]. The photo-physics of plasmonics and PL effect are not well understood in ensemble measurements. The understanding of the size and surface effect are essentially important from the further integration of these nanoparticles with other nanosystems to utilize their modified optical properties. In this work, we want to address the size effect of these systems especially weakly coupled gold (Au) nanoparticles by tunneling spectroscopy. Differential conductance of individual noble metal nanoparticles with different temperatures (from mK to K order) shows band-structure fluctuations which can effectively provide signature information of the nanoparticles. We discuss our results in terms of correlations between the electron dynamics, size, surface functionalization and temperature.

[1] S. Eustisa, M. A. El-Sayed, Chem. Soc. Rev. **35**, 209 (2006)
[2] J. Zheng, C. Zhou, M. Yua, J. Liua, Nanoscale **4**, 4073 (2012).

TT 55: Frontiers of Electronic Structure Theory: Focus on Topology and Transport III (Joint session of DS, HL, MA, MM, O and TT organized by O)

Time: Wednesday 15:00–18:30 Location: H24

Topical Talk TT 55.1 Wed 15:00 H24

Topological semimetal phases in strained HgTe-based alloys — Tomáš Rauch[1], Steven Achilles[1], •Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

Topological insulators (TIs) have matured to a class of materials that is studied worldwide with great effort. Prominent examples are HgTe, the Bi chalcogenides, and SnTe. Recently, the set of "original" TIs has been extended by topological semimetals: the topological Dirac and the Weyl semimetals, both of them showing point-like Fermi surfaces in the bulk. Weyl points appear always in pairs with opposite topological charges of ± 1; their projections onto the surface Brillouin zone are connected by a Fermi arc, i. e. a sizably spin-polarized topological surface state with an open Fermi contour.

In this presentation I report on theoretical investigations of strained $HgTe_{1-x}S_x$ alloys [1], with surprising results. (*i*) In the strong TI phase, the spin chirality of the topological nontrivial surface state can be reversed by moderate strain and changing the alloy concentration x. (*ii*) On top of this, we observe a Dirac and a Weyl semimetal phase. These findings call for experimental verification and extend significantly the "topological playground" for spin-dependent transport.

[1] T. Rauch, S. Achilles, JH, I. Mertig, Phys. Rev. Letters **114** (2015) 236805.

Topical Talk TT 55.2 Wed 15:30 H24

Topological surface Fermi arcs and the chiral anomaly in Weyl semimetal materials — •Binghai Yan — Max Planck Institute for Chemical Physics of Solids, Dresden

Topological Weyl semimetals represent a novel state of topological quantum matter, which not only possesses Weyl fermions (massless chiral particles that can be viewed as magnetic monopoles in momentum space) in the bulk and unique Fermi arcs generated by topological surface states, but also exhibits appealing physical properties such as extremely large magnetoresistance and ultra-high carrier mobility. In this talk, I will first present our recent theoretical [1] and ARPES [2,3] study on the topological surface states of transition-metal monopnictides, NbP, NbAs, TaP and TaAs. By visualizing the surface Fermi arcs, we discovered their Fermiology evolution with spin*orbit coupling strength. Further, we found a way to manipulate the Fermi arcs by the Lifshitz transition. I will also introduce our recent progress on the magneto-transport in the search for the chiral anomaly effect[4,5]. References: [1] Y. Sun, S. C. Wu, and B. Yan, Phys. Rev. B 92, 115428 (2015). [2] L. X. Yang, et al. Nature Physics 11, 728 (2015). [3] Z. K. Liu, et al. Nature Materials DOI: 10.1038/NMAT4457 (2015). [4] C. Shekhar, et al. Nature Physics 11, 645 (2015). [5] C. Shekhar, et al. arXiv:1506.06577 (2015).

TT 55.3 Wed 16:00 H24

Type-II Dirac cones as unified topological origin of the exotic electronic properties of WTe_2 — •Lukas Muechler[1], Aris Alexandradinata[2], Titus Neupert[3], and Roberto Car[1] — [1]Dept. of Chemistry, Princeton University — [2]Dept. of Physics, Yale University — [3]Princeton Center for Theoretical Science, Princeton University

WTe_2 is a recently discovered layered material with remarkable electronic properties. Transport measurements show an extremely large non-saturating magnetoresistance (MR) with mobilities as high as 167 000 cm^2/Vs at 2 K. Furthermore, recent photoemission experiments discovered circular dichroism in the bulk band structure. We propose a unified explanation for these exotic observations by relating key properties of the bulk electronic structure to that of to that of the mono- and bi-layer material. In particular, we demonstrate that the monolayer is a novel type-II Dirac semimetal in absence of spin-orbit coupling, with Dirac cones that are sufficiently anisotropic to simultaneously harbor electron and hole pockets. The band structure can be characterized by a new $\mathbb{Z}_2 \times \mathbb{Z}_2$ topological invariant defined through non-Abelian Wilson loops. We develop a tight-binding model for the mono- and bilayer of WTe_2 based on Wannier functions from *ab-inito* calculations and extend our findings to the iso-structural compounds $MoTe_2$ and ZrI_2.

TT 55.4 Wed 16:15 H24

Topological surface Fermi arcs and spin-textures of the Weyl semimetals TaAs, TaP, NbAs, and NbP — •Yan Sun[1], Shu-Chun Wu[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany. — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Very recently the topological Weyl semimetal (WSM) was predicted in the noncentrosymmetric compounds NbP, NbAs, TaP, and TaAs and soon led to photoemission experiments to verify the presumed topological Fermi arcs (FAs)[1,2]. In this work we have performed fully ab initio calculations of these four WSMs and revealed the FAs with spin-momentum-locked spin texture[3]. On the (001) surface, the anion (P or As) terminated surfaces are found to fit photoemission measurements well. By tracing the spin polarization of the Fermi surface, one can distinguish FAs from trivial Fermi circles. By comparing their surface states, we reveal the evolution of topological Fermi arcs from the spin-degenerate Fermi circle to spin-split arcs when the SOC increases from zero to a finite value. Our work presents a comprehensive understanding of the topological surface states of WSMs, which will be helpful for spin-revolved photoemission and transport experiments.

References

[1] L. X. Yang, Z. K. Liu, Y. Sun, et. al. Nat.Phys.11,728, (2015).

[2] Z. K. Liu, L. X. Yang, Y. Sun, et.al Nat. Mater., doi:10.1038/nmat4457,(2015).

[3] Y. Sun, S. Wu, and B. Yan, Phy. Rev. B, 92, 115428, (2015).

TT 55.5 Wed 16:30 H24

New electron states at the Bi/InAs(111) interface — •L Nicolaï[1,2,3], K Hricovini[2,3], J-M Mariot[4], M C Richter[2,3], O Heckmann[2,3], U Djukic[2], T Balasubramanian[5], M Leandersson[5], J Sadowski[5], J Denlinger[6], I Vobornik[7], J Braun[7], H Ebert[7], and J Minár[7,8] — [1]LMU, Munich — [2]LPMS, UCP, Cergy, France — [3]DSM-IRAMIS, Spec, Cea-Saclay, France — [4]LCP-MR, UPMC Univ. Paris 06/CNRS, France — [5]MAX-lab, Lund Univ., Sweden — [6]ALS, Berkeley, USA — [7]EST, Trieste, Italy — [8]Univ. of West Bohemia, Plzeň, Czech Republic

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] M. Wada et al., Phys. Rev. B 83, 121310 (2011). [2] Z. Liu et al., Phys. Rev. Lett. 107, 136805 (2011). [3] J. Braun, Rep. Prog. Phys. 59, 1267-1338 (1996).

TT 55.6 Wed 16:45 H24

Two-dimensional topological phases and electronic spectra of topological insulator thin films from *GW* calculations — •Tobias Förster, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

We have investigated topological and electronic properties of thin films of the topological insulators Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3 with thicknesses from one to six quintuple layers employing the *GW* method. The quasiparticle band structures show highly improved agreement with experiments compared to DFT. In addition to a correction of the band gaps, the energetic positions and dispersions of the surface states change significantly around $\bar{\Gamma}$ [1]. The common approach of taking the diagonal elements of the self-energy Σ as quasiparticle energies and leaving the wave functions unchanged yields unphysical results which can be overcome by diagonalizing $\mathcal{H}^{\mathrm{QP}}$. The origin of the respective

off-diagonal elements in $(\Sigma - V_{xc})$ will be discussed. As the wave functions are updated, the two-dimensional topological phases (quantum spin Hall or trivial) in *GW* differ from DFT for many systems. On the basis of our results, we further argue that one cannot unambiguously conclude the topological phase from fits to ARPES band structures as performed in recent experimental studies.

[1] T. Förster, P. Krüger, and M. Rohlfing, Phys. Rev. B **92**, 201404(R) (2015)

TT 55.7 Wed 17:00 H24

Steady-State Density Functional Theory for Finite Bias Conductances — •Stefan Kurth[1,2] and Gianluca Stefanucci[3,4] — [1]Dept. of Materials Physics, Univ. of the Basque Country UPV/EHU, San Sebastian, Spain — [2]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [3]Dept. of Physics, Univ. of Rome "Tor Vergata", Rome, Italy — [4]INFN, Frascati, Italy

In the framework of density functional theory a formalism to describe electronic transport in the steady state is proposed which uses the density on the junction and the steady current as basic variables. In a finite window around zero bias, a one-to-one map is established between the basic variables and both local potential on as well as bias across the junction. The resulting Kohn-Sham system features two exchange-correlation (xc) potentials, a local xc potential and an xc contribution to the bias. For weakly coupled junctions the xc potentials exhibit steps in the density-current plane which are shown to be crucial to describe the Coulomb blockade diamonds. At small currents these steps emerge as the equilibrium xc discontinuity bifurcates. The formalism is applied to a model benzene junction, finding perfect agreement with the orthodox theory of Coulomb blockade.

TT 55.8 Wed 17:15 H24

Revealing the intra-molecular origin of inelastic electron tunneling signal by means of first-principles calculations — •Giuseppe Foti and Hector Vazquez — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, Prague, Czech Republic

We explore the intra-molecular contributions to the peaks in the Inelastic Electron Tunneling Spectrum (IETS) of a benzene-based molecular junction by means of DFT-NEGF simulations [1,2]. These contributions are calculated from the bracket of the left- and right- transmission channels with the e-ph coupling matrix by grouping the products into one- and two-atom terms. This combines the geometrical information of the vibrational modes with the electronic properties of the scattering states. Our calculations show how the partial contributions of each atom and bond in the molecule combine to give the total inelastic signal. We find that, for most of the high intensity peaks, these terms sum up constructively while dark modes result from cancellations. We also investigate the relation between the symmetry of the vibrational modes and the cancellation pattern of the different contributions. This analysis enables a real space representation of the intra-molecular contributions associated to each vibrational mode and allows a complete mapping and characterization of the origin of the IETS peaks.

[1] J. M. Soler et al. J. Phys.: Condens. Matter 14, 2745 (2002)
[2] T. Frederiksen et al. Phys. Rev. B 75, 205413 (2007)

TT 55.9 Wed 17:30 H24

An efficient real-time time-dependent density functional theory method and its applications — •Zhi Wang[1], Shu-Shen Li[2], and Lin-Wang Wang[3] — [1]Institut für Physikalische Chemie, Uni-Hamburg, Hamburg, Germany — [2]Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China — [3]Lawrence Berkeley National Laboratory, Berkeley, United States

We have developed an efficient real-time time-dependent density functional theory (TDDFT) method that can increase the effective time step from <1 as in traditional methods to ~0.1 fs. With this algorithm, the TDDFT simulation can have comparable speed to the Born-Oppenheimer (BO) ab initio molecular dynamics (MD). The application of the method will be illustrated for several non-equilibrium systems, e.g., energetic particle colliding onto a TMDC monolayer, and ultrafast charge seperations in photovoltaic systems.

TT 55.10 Wed 17:45 H24

Nonadiabatic geometric phase of a pseudorotating triatomic molecule — •Ryan Requist and Eberhard K. U. Gross — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The geometric phase of a real-valued Born-Oppenheimer electronic wavefunction is a topological quantity depending on the winding number of the path around a conical intersection of the adiabatic potential energy surfaces in nuclear coordinate space. We report the calculation of a nonadiabatic molecular geometric phase that takes the full quantum mechanical motion of the nuclei into account through the exact factorization scheme [1]. Nonadiabatic contributions "smear out" the point-like adiabatic Berry curvature, changing the topological invariant into a genuine path-dependent geometric phase [2].

[1] S. K. Min, A. Abedi, K. S. Kim and E. K. U. Gross, Phys. Rev. Lett. 113, 263004 (2014). [2] R. Requist and E. K. U. Gross, arxiv:1506.09193.

TT 55.11 Wed 18:00 H24

Theoretical investigations of magnetically doped topological insulators — •Jan Minar[1,2], Jurgen Braun[1], and Hubert Ebert[1] — [1]LMU München, Germany — [2]University of West Bohemia, Plzen, Czech Rep.

Band gap opening of topological surface states due to magnetic doping are the subject of a long standing 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. Here we will present several examples detailed theoretical studies on various bulk as well as surface doped topological insulators by means of the SPR-KKR band structure method. Our results will be discussed in a direct comparison with the corresponding ARPES [1] as well as XAS and XMCD [2,3] experimental data.

[1] J. Sanchez-Barriga et al., Nat. Communications, submitted (2015) [2] A. Ney et al., in preparation [3] J. Honolka et al., in preparation

TT 55.12 Wed 18:15 H24

Trions in a carbon nanotube from ab-initio many-body perturbation theory — •Thorsten Deilmann, Matthias Drüppel, and Michael Rohlfing — Institut für Festkörpertheorie, Universität Münster, Germany

Trion states of three correlated particles (e.g. two electrons and one hole) show up in the optical spectra of doped or gated nanostructures, like carbon nanotubes or transition-metal dichalcogenides.
We demonstrate that trions can be described within ab-initio many-body perturbation theory, as a natural extension of the widely used *GW* method and Bethe-Salpeter equation. This allows for a direct comparison with excitons on equal footing.
We investigate trion states in a semiconducting $(8, 0)$ carbon nanotube, and discuss their spectra, composition, and wave functions. Luminescence from the trions is red-shifted by $\sim 135\,\text{meV}$ compared to the excitons.

TT 56: Graphene: Adsorption, Intercalation and Doping (Joint session of DS, DY, HL, MA, O and TT organized by O)

Time: Wednesday 15:00–18:00 Location: S053

TT 56.1 Wed 15:00 S053

H atom scattering from epitaxial graphene on Pt(111) — •Hongyan Jiang[1], Yvonne Dorenkamp[1], Alec Wodtke[1,2,3], and Oliver Buenermann[1,2,3] — [1]Institute for Physical Chemistry, Georg-August University of Goettingen, Goettingen, Germany — [2]Department of Dynamics at Surfaces, Max Planck Institute for Biophysical Chemistry, Goettingen, Germany — [3]International Center for Advanced Studies of Energy Conversion, Georg-August University of Goettingen, Goettingen, Germany

Adsorption of hydrogen atoms on graphene is playing an important role in hydrogen storage, graphene based electronics, nuclear fusion and interstellar chemistry. The interaction of hydrogen atoms with

graphene is studied in a newly built atom-surface scattering machine. A nearly mono-energetic hydrogen atom beam is formed by laser photolysis. The hydrogen atoms are scattered from a well-defined sample held in UHV. The scattered hydrogen atoms are detected using Rydberg-atom neutral time-of-flight. This technique allows us to record angle resolved, high resolution energy loss spectra of scatted hydrogen atoms. Scattering of hydrogen atoms from epitaxial graphene on Pt(111) shows a very different behavior than scattering from clean Pt(111). For low incidence kinetic energy, graphene acts like an atomic mirror. We observe narrow scattering angle and kinetic energy distribution and small translational energy loss. For high incidence kinetic energy, broad distribution and large translational energy loss is observed. The process obeys normal energy scaling. We speculate that this behavior is connected to the barrier of hydrogen atom adsorption on graphene.

TT 56.2 Wed 15:15 S053

A nanodiamond superlattice on graphene/Ir(111) — •Charlotte Herbig[1], Philipp Valerius[1], Timo Knispel[1], Sabina Simon[1,2], Ulrike A. Schröder[1], Antonio J. Martínez-Galera[1], Mohammad A. Arman[3], Christian Teichert[1,4], Jan Knudsen[3,5], Arkady V. Krasheninnikov[6,7], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Department of Physics, University of Konstanz, Germany — [3]Division of Synchrotron Radiation Research, Lund University, Sweden — [4]Institute of Physics, Montanuniversität Leoben, Austria — [5]MAX IV Laboratory, Lund, Sweden — [6]Department of Applied Physics, Aalto University, Finland — [7]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany

Atomic C deposition onto the graphene moiré with Ir(111) leads in a broad temperature range from 130 K to 550 K to the formation of a nanodiamond superlattice with one C cluster per moiré unit cell. The size of the C clusters is tunable between about 20 and 150 C atoms. For deposited amounts exceeding about 200 C atoms per moiré unit cell the ordering is lost, but still nanodiamond structures remain. The nanodiamond superlattice is thermally stable up to 800 K. Annealing to higher temperatures results in C intercalation and eventually bilayer graphene formation. On the basis of scanning tunneling microscopy, X-ray photoelectron spectroscopy, and density functional theory a model for C cluster formation, structure, stability, and decay is developed. Based on the generality of our model, we speculate that nanodiamonds may form on other moirés of 2D materials with their substrate.

TT 56.3 Wed 15:30 S053

Core level shifts of doped graphene — •Ulrike A. Schröder[1], Marin Petrović[2], Timm Gerber[1], Elin Grånäs[3], Antonio J. Martínez-Galera[1], Mohammad A. Arman[3], Charlotte Herbig[1], Joachim Schnadt[3], Marko Kralj[2], Jan Knudsen[3,4], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut za fiziku, Zagreb, Croatia — [3]Division of Synchrotron Radiation Research, Lund University, Sweden — [4]MAX IV Laboratory, Lund, Sweden

In X-ray photoemission spectroscopy, core level shifts of the carbon 1s photoelectrons are frequently monitored to investigate adsorption and intercalation on and underneath graphene. An understanding of their origin and magnitude are thus desirable both from a scientific and an applicational point of view. Through intercalation of metals and gases, the Dirac cone of graphene on Ir(111) can be shifted with respect to the Fermi level without becoming destroyed through strong hybridization. Upon such chemical doping with Cs, Eu, H, O, and Li, the carbon 1s core level shift displays a functional dependence on the graphene doping level. Of specific interest is the case of doping by Li, since for Li no phase separation takes place upon intercalation. Thereby, this core level shift can be monitored as a function of the intercalated amount. To first approximation, the core level shift may be described as a superposition of a rigid band shift, which is counteracted by a shift proportional to the transferred charge.

TT 56.4 Wed 15:45 S053

Structural phases of Au-intercalated graphene on Ni(111) — •Maxim Krivenkov[1,2], Evangelos Golias[1], Dmitry Marchenko[1], Jaime Sánchez-Barriga[1], Gustav Bihlmayer[3], Oliver Rader[1], and Andrei Varykhalov[1] — [1]Helmholtz-Zentrum Berlin, BESSY-II, 12489, Berlin, Germany — [2]Department of Physics, Potsdam University, Am Neuen Palais 10, D-14415, Potsdam, Germany — [3]Forschungszentrum Jülich and JARA, 52425, Jülich, Germany

Graphene grown epitaxially on Ni(111) and intercalated with Au is a remarkable system revealing a giant (∼100 meV) spin-orbit splitting of Dirac cone in spin-resolved photoemission experiments [1]. In present study we investigate structural origin of this giant Rashba effect. We report extensive microscopic study of Au-intercalated graphene and discover versatile structural phases of Au locally coexisting at graphene-Ni interface. Besides a continuous monolayer phase giving rise to a pronounced moiré pattern identified as (9.7×9.7) misfit dislocation loop structure [2], we observe various well periodic arrays of nanoparticles trapped under graphene. Overall arrangement of such Au nanoclusters is laterally coherent to the principle moiré pattern of Au monolayer. We test whether these nanoparticles can be a source of giant spin-orbit splitting in graphene by performing DFT study of structural and electronic properties of the system.

[1] D. Marchenko, A. Varykhalov, M. R. Scholz, G. Bihlmayer, E. I. Rashba, A. Rybkin, A. M. Shikin, O. Rader, Nature Commun. 3, 1232 (2012); [2] J. Jakobsen et al., Phys. Rev. Lett. 75, 489 (1995).

TT 56.5 Wed 16:00 S053

How to manipulate the dispersion interaction at organic-graphene interfaces — •Vasile Caciuc[1], Felix Huttmann[2], Nicolae Atodiresei[1], Thomas Michely[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

In this contribution we will explore how to rationally engineer the strength of the van der Waals (vdW) interactions present in a molecule–surface physisorbed system. More specifically, we investigated by means of *ab initio* density functional theory (DFT) simulations using a non-local correlation vdW functional [1] the adsorption of a $\pi-$conjugated organic molecule such as naphthalene ($C_{10}H_8$) on the graphene/Ir(111) surface [2]. To tailor the magnitude of the naphthalene–graphene dispersion interaction, the key ingredient is to modify the spatial extent of the charge distribution in graphene by doping it via intercalated electropositive and electronegative atoms at its backside to Ir(111) [3]. Finally, the comparison of the predicted adsorption energies and those obtained by thermal desorption measurements is also discussed [4].

[1] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004).
[2] C. Busse *et al.*, Phys. Rev. Lett. **107**, 036101 (2011).
[3] S. Schumacher *et al.*, Nano Lett. **13**, 5013 (2013).
[4] F. Huttmann *et al.*, Phys. Rev. Lett., accepted.

TT 56.6 Wed 16:15 S053

Coverage dependent evolution of electronic states of tetraphenyldibenzoperiflanthene (DBP) on HOPG and graphite — •Tobias Huempfner[1], Tino Kirchhuebel[1], Roman Forker[1], Noriaki Kawakita[2], Takashi Yamada[2], Toshiaki Munakata[2], and Torsten Fritz[1,2] — [1]Friedrich Schiller University, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]Department of Chemistry, Graduate School of Science, Osaka University, 1-1 Machikaneyama, Toyonaka 560-0043, Osaka, Japan

We report on a combined study of the dye molecule tetraphenyldibenzoperiflanthene (DBP) deposited on HOPG and single crystalline graphite surfaces. The film growth is successively traced in situ via differential reflectance spectroscopy (DRS). This data is compared to ultraviolet photoelectron spectroscopy (UPS) as well as two photon photoemission (2PPE) measurements recorded at various coverages. All methods applied show that there are two different species of the DBP molecule that appear at certain film thicknesses. For low coverages, namely up to one monolayer (ML), the absorption gap of the molecules is smaller (low energy - LE) compared to coverages slightly above 1 ML (high energy - HE). For thicker films up to 10 ML the LE species is formed again and the film composition shifts continuously in favor of this species with increasing coverage. This study is assisted by structural data gained from low energy electron diffraction (LEED) and scanning tunneling microscopy (STM) that depicts a highly ordered first ML.

TT 56.7 Wed 16:30 S053

Supramolecular nanopatterns of organic molecules on graphite — •Stefan-Sven Jester — Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn

The self-assembly of organic molecules at the solid/liquid interface provides an approach towards defined 2D architectures. However, pre-

dicting how a specific molecule renders into a supramolecular 2D crystal is still a challenge. A promising approach relies on the transfer of concepts from discrete geometry (e.g. Archimedean surface tiling) to supramolecular chemistry: Arylene-alkynylene macrocycles of distinct symmetries and sizes that carry flexible alkyl/alkoxy side chains can be viewed as molecular polygons that form supramolecular patterns of specific symmetries and lattice constants. E.g., the cocrystal of molecular triangles and hexagons has increased lattice constants as compared to the individual compounds. We describe a concentration-driven alteration between porous and dense packings of hexagons with reduced symmetry and alike unit cell parameters for rings with different interiors. In addition, we discuss mono- and multilayer growth of molecular spoked wheels on graphite. In all cases, scanning tunneling microscopy provides a submolecularly resolved insight into the molecular structures that can be utilized for chemical compound analysis.

TT 56.8 Wed 16:45 S053

Molecular friction and proton dynamics in sulfuric acid intercalated graphite from ab-initio MD simulations — •Steffen Seiler and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Wet-chemical exfoliation of graphite via Hummers' method [1,2] is a promising route for large-scale graphene production. In this solution-based process first graphite is intercalated by concentrated sulfuric acid, then the graphite intercalation compound (GIC) is oxidized, graphene oxide (GO) layers are separated in solution by hydrolysis reactions, and finally the GO layers are reduced to graphene [3].
We performed Car-Parrinello molecular dynamics (CP-MD) simulations to study the dynamic properties of the liquid sulfuric acid within the confined space between the graphene layers. The friction coefficient, proton-transfer barriers and electron distributions have been analyzed, and we will show how these properties are affected by the oxidation and the stacking sequence of the graphene sheets. Finally, consequences for the mechanism of GIC formation and oxidation will be discussed.

[1] W. S. Hummers, *J. Am. Chem. Soc.* **80**, 1339 (1958).
[2] D. C. Marcano et al., *ACS Nano* **4**, 4806 (2010).
[3] A. M. Dimiev and J. M. Tour, *ACS Nano* **8**, 3060 (2014).

TT 56.9 Wed 17:00 S053

Surface mediated oxidation of supported coronene molecules — •Weippert Jürgen[1], Gewiese Vincent[1], Böttcher Artur[1], and Kappes Manfred M.[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 explored surface-mediated oxidation of coronene (C24H12) molecules as a route to prepare molecular equivalents of graphene oxides (GOs). We found that exposure of C24H12/HOPG to a flux of atomic oxygen leads to oxidation of both the substrate and the coronene molecules adsorbed thereon (O/HOPG and C24H12On). We did not observe molecular fragments indicative of epoxy-species induced unzipping and scission of the adsorbed coronene. Instead desorption mass spectra were dominated by Coronene molecules deriving from electron impact ionization of the intact parent species, two oxidic species and an unusual coronene fragment, C21H9+. These observations suggest that sample heating activates the surface diffusion of preformed epoxy species and that subsequently pronounced fragmentation of the oxidized molecular periphery is induced either by further on-surface heating or by ionization. The reaction path results in the emission of coronene oxides with a mean yield of 0.07. Systematic measurements (TDS, UPS and XPS) reveal further details of the reaction chain associated with efficient thermal desorption of coronene oxides - a process analogous to the exfoliation of graphene oxide.

TT 56.10 Wed 17:15 S053

Intercalation of Gadolinium underneath graphene on SiC(0001) — •Stefan Link, Stiven Forti, Alexander Stöhr, and Ulrich Starke — Max-Planck-Institut für Festkörperforschung Stuttgart

Tuning the electronic properties of graphene for potential applications has raised intensive research. Besides spatial confinement for the introduction of a band gap or covalent functionalization, the intercalation of foreign atom species is a promising approach. A highly interesting state of graphene lies in the extreme doping regime, where a van-Hove singularity is reached at the Fermi level. Although this is a rather difficult task, it might pave the way to introduce interesting effects like superconductivity. Gating is illusional for this purpose due to the lack of appropriate dielectrica. Notably, the introduction of dopant adatoms like alkali and/or earth alkali metals onto both sides of the graphene leads to success but on the cost of strongly reduced stability. Here we show in a different approach that such a system can be produced with strong thermal and chemical stability. The system develops by intercalating Gadolinium atoms beneath the so called zerolayer graphene on SiC(0001). We make use of the advanced fabrication of epitaxial graphene on SiC(0001) in our group to achieve homogeneous results on a large scale. This gives the opportunity for exploring graphene's properties in this exotic regime. We show that reaching this regime is accompanied by strong renormalization effects in the electronic band structure, which are partially driven by strong electron-phonon coupling.

TT 56.11 Wed 17:30 S053

Transformation of metallic boron into substitutional dopants in graphene on 6H-SiC(0001) — •Jessica Sforzini[1,2], Mykola Telychko[3,4], Ondrej Krejcio[3,4], Martin Vondracek[5], Martin Svec[3], Francois Bocquet[1,2], and Stephan Tautz[1,2] — [1]Peter Gruenberg Institut (PGI-3), Forschungszentrum Juelich, 52425 Juelich, Germany — [2]Juelich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, 52425 Juelich, Germany — [3]Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, CZ-16200 Prague, Czech Republic — [4]Faculty of Mathematics and Physics, Charles University, V Holesovickach 2, Praha 8, Czech Republic — [5]Institute of Physics, Academy of Science of the Czech Republic, Na Slovance 2, 10, CZ-18228 Prague, Czech Republic

We investigate the development of the local bonding and chemical state of boron atoms during the growth of B-doped graphene on 6H-SiC(0001). Photoemission experiments reveal the presence of two chemical states, namely boron in the uppermost SiC bilayers and boron substituted in both the graphene and buffer layer lattices. We demonstrate the participation of the dopant in the π^* electron system of graphene by the presence of the π^* resonance in the near edge x-ray adsorption fine structure (NEXAFS) recorded at the B K-edge. The experimental fundings are supported by NEXAFS simulations.

TT 56.12 Wed 17:45 S053

Chemical modification of bilayer graphene — •Konstantin Weber and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Using density functional theory (DFT) together with the empirical Grimme D2 van der Waals correction scheme [1] we studied the energetics, reaction pathway and thermodynamics of the hydroxylation and hydrogenation reaction and subsequent interlayer bond formation in bilayer graphene. Our results show that after the adsorption of two to three adsorbates a critical nucleous size is reached and subsequent adsorption leads to an energy gain for both the adsorption of hydrogen and hydroxyl groups. The covalent adsorption increases the reactivity of bilayer graphene and triggers the formation of interlayer bonds between the graphene sheets. In addition, the reactivity of freestanding bilayer graphene will be compared to the reactivity of bilayer graphene adsorbed on a Ni(111) substrate. The Ni(111) surface acts as a support and reaction template that facilitates the hydrogenation and hydroxylation reactions, similarly as in the one-sided hydrogenation process of single-layer graphene supported on Ni(111) [2].

[1] S. Grimme, *J. Comp. Chem.* **27**, 1787 (2006).
[2] W. Zhao et al., *Chem. Eur. J.* **21**, 3347 (2015).

TT 57: Topological Insulators (Joint session of MA, DS, HL, O and TT organized by MA)

Time: Wednesday 15:00–17:45 Location: H32

TT 57.1 Wed 15:00 H32

Bulk and surface properties of topological insulators from *GW* calculations. — •Irene Aguilera, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany.

Many-body calculations within the *GW* approximation are attracting much attention in the study of topological insulators (TIs). They have shown to be critical both in the one-shot approach [1] (e.g. for the Bi_2Se_3 family) and in a quasiparticle self-consistent (QS) *GW* method [2] (e.g. for Bi). In both cases, the spin-orbit coupling has to be incorporated directly into the *GW* self-energy [3]. Within the all-electron FLAPW formalism, we have performed DFT, one-shot *GW*, and QS*GW* calculations for well-known TIs. These calculations are very demanding for low-dimensional systems. Therefore, we construct a tight-binding Hamiltonian for the description of topological surface states in a slab geometry. The corresponding parameters are deduced from *GW* calculations of the bulk. With this approach, we discuss the effects of quasiparticle corrections on the surface states of TIs and on the interaction between bulk and surface states. We show that the *GW* bulk and surface band structure agrees better to results from photoemission experiments than the DFT one. [1] Phys. Rev. B 87, 121111(R) (2013). [2] *Ibid* 91, 125129 (2015). [3] *Ibid* 88, 165136 (2013).

We acknowledge the Virtual Institute for Topological Insulators of the Helmholtz Association.

TT 57.2 Wed 15:15 H32

Magnetic Properties of Mn-doped Bi_2Se_3 and Bi_2Te_3: Ab Initio and Atomistic Simulations — •Pavel Baláž[1], Karel Carva[1], Róbert Tarasenko[1], Vladimír Tkáč[1], Jan Honolka[2], and Josef Kudrnovský[2] — [1]DCMP, Charles University, Ke Karlovu 5, CZ-12116 Prague 2, Czech Republic — [2]Institute of Physics, ASCR, Na Slovance 2, CZ-18221 Prague 8, Czech Republic

Ferromagnetic Curie temperature and other magnetic magnetic properties of bulk Mn-doped Bi_2Se_3 and Bi_2Te_3 3D topological insulators are systematically studied by means of atomistic Monte Carlo simulations. Exchange interactions between the Mn magnetic moments have been calculated using ab initio methods. Tight-binding linear muffin-tin orbital method has been employed, together with the coherent potential approximation to describe the high degree of disorder in the system. Spin-orbit interaction is included in the ground state calculation. In the studied materials Mn atoms might either replace a Bi atom (substitutional position) or fill an empty position in van Der Waals gap between the atomic layers (substitutional position). It has been shown that exchange interaction between Mn magnetic moments might lead to a ferromagnetic phase transition. The Curie temperature is shown to be significantly dependent on the concentration of Mn atoms in substitutional and interstitial positions. Theoretical results were compared to recent experimental studies [1].

[1] R. Tarasenko et al., to be published in Physica B: Phys. Cond. Mat., DOI: 10.1016/j.physb.2015.11.022

TT 57.3 Wed 15:30 H32

Transport measurements on ferromagnet / Half Heusler TI bilayer structures — •Benedikt Ernst[1], Robin Klett[2], Jan Haskenhoff[2], James Taylor[3], Yong Pu[3], Günter Reiss[2], Stuard S. P. Parkin[3], and Claudia Felser[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden — [2]Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld — [3]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle

Heusler compounds exhibit a manifold of physical properties and attracted in the recent past a lot of interest in the field of spintronic applications due to their half-metallic properties.

In the present work bilayer systems of ferromagnetic materials and half Heusler topological insulators (TI) are studied. The systems were deposited using DC- and RF magnetron co-sputtering. The samples were characterized by X-ray diffraction and electron microscopy techniques. On fabricated devices, the transport properties and spin properties were studied by different measurement techniques including ST-FMR and spin injection experiments.

Additional measurements of the unidirectional spin Hall magnetoresistance were realized. In this effect, we measure a change in the magnetoresistance depending on the direction of the magnetization, which is proportional to the spin Hall angle. We varied the combination of different ferromagnetic materials with different Tis of the YPtBi, YPdBi, LaPtBi and LaPdBi system, and the thicknesses of the layers, to investigate the effects on the transport properties.

TT 57.4 Wed 15:45 H32

Surface preparation and momentum microscopy of the „topological Kondo insulator“ SmB_6 — •Christian Tusche[1,2], Martin Ellguth[1], Fumitoshi Iga[3], and Shigemasa Suga[2,4] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]College of Science, Ibaraki University, Japan — [4]Institute of Scientific and Industrial Research, Osaka University, Osaka, Japan

The strongly correlated rare-earth compound SmB_6 is believed to be a topological Kondo insulator, where a topologically non-trivial surface state lives in the hybridization gap at low temperatures. While most experimental studies rely on cleaved surfaces, high resolution- and spin resolved photoemission experiments [1] usually suffer from the short live time of the reactive surface at low temperatures.

Here we present the reproducible surface preparation of large high quality SmB_6 single crystals by in-situ Ar-ion sputtering and controlled annealing. In particular, Sm-rich or B-rich surface terminations are obtained by low (≈1080°C) or high (>1200°C) temperature annealing. Using a momentum microscope [2], wide wave vector regions are studied by photoemission with He-I ($h\nu$=21.2 eV) and laser ($h\nu$=6.0 eV) excitations, on the Sm-terminated surface. The results reveal localized f-electron resonances at E_F and strong hybridization, paving the way to measure detailed Fermi surface and valence band spin textures.

[1] Suga et al., J., Phys. Soc. Japan 83, 014705 (2014)
[2] C. Tusche, A. Krasyuk, J. Kirschner, Ultramicroscopy (2015)

TT 57.5 Wed 16:00 H32

Spin control in the topological surface state of SnTe — •Nicolas Klier[1], Sam Shallcross[1], Sangeeta Sharma[2], and Oleg Pankratov[1] — [1]Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7-B2, 91058 Erlangen — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

The interface of SnTe with a vacuum results in a topological Dirac surface state [1,2]. Based on an effective Hamiltonian derived from tight-binding we investigate the properties of this surface state both with and without an in-plane electric current. The RKKY interaction is found to be strongly non-collinear due to the spin texture of the Dirac state. In the presence of an in-plane current we find (i) a polarization of the surface state and (ii) that the RKKY interaction is strongly modified by the presence of a current leading to a possible “topological spin torque effect”.

[1] B.A. Volkov, and O.A. Pankratov, Zh.Eksp. Theor. Fiz. 75, 1362, 1978.
[2] B.A. Volkov, and O.A. Pankratov, JETP Lett.42, 178, 1985.

15 min. break

TT 57.6 Wed 16:30 H32

Adiabatic Pumping of Chern-Simons Axion Coupling — •Maryam Taherinejad[1] and David Vanderbilt[2] — [1]Materials Theory, ETH Zurich, Wolfgang-Pauli-Strasse 27, 8093 Zurich, Switzerland — [2]Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854-0849, USA

The Chern-Simons axion (CSA) coupling θ makes a contribution of topological origin to the magnetoelectric response of insulating materials. Here we study the adiabatic pumping of the CSA coupling along a parametric loop characterized by a non-zero second Chern number $C^{(2)}$ from the viewpoint of the hybrid Wannier representation. The hybrid Wannier charge centers (WCCs), when plotted over the 2D projected Brillouin zone, were previously shown to give an insightful visualization of the topological character of a 3D insulator. By defining Berry connections and curvatures on these WCC sheets, we de-

rive a new formula for θ, emphasizing that it is naturally decomposed into a topological Berry-curvature dipole term and a nontopological correction term. By explicit calculations on a model tight-binding Hamiltonian, we show how the Berry curvature on the WCC sheets is transported by a lattice vector via a series of Dirac sheet-touching events, resulting in the pumping of e^2/h units of CSA coupling during one closed cycle. The new formulation may provide a particularly efficient means of computing the CSA coupling θ in practice, since there is no need to establish a smooth gauge in the 3D Brillouin zone.

TT 57.7 Wed 16:45 H32

Accessing the transport limits of topological states — •Thomas Bathon[1], Paolo Sessi[1], Konstantin Kokh[2], Oleg Tereshchenko[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Novosibirsk State University, 630090 Novosibirsk, Russia

Topological insulators host on their surface spin-momentum locked Dirac states. Beyond their fundamental interest, these materials raised great expectations to create new functionalities in spintronics and magneto-electrics. Their success depends on our understanding of their response to Coulomb perturbations such as electric fields, which can be effectively used to gate their surface. These phenomena have so far been primarily explored by spatially averaging techniques.

Here, by using scanning tunneling microscopy and spectroscopy, we visualize the response of topological states to local charges and electric fields at the nanoscale. We demonstrate that, contrary to the general believe, local electric fields can not be effectively screened by topological states, but penetrate into the bulk indicating a behavior which is far from being metallic. The analysis of our data allows to detect the existence of a finite conductivity which, because of the local character of our measurements, can be safely quantified without being affected by sample inhomogeinities. Finally, we will show how, by taking advantage of this intrinsic limitation, a new approach to tune both charge and spin transport in this fascinating class of materials can be explored.

TT 57.8 Wed 17:00 H32

Interplay between warping and magnetic effects in Fe monolayer on Sb2Te3 — •Farideh Hajiheidari[1], Wei Zhang[1,2], and Riccardo Mazzarello[1,3] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52074 Aachen, Germany — [2]Center for Advancing Materials Performance from the Nanoscale, State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, PR China — [3]JARA-FIT and JARA-HPC, RWTH Aachen University, D-52074 Aachen, Germany

Three-dimensional topological insulators (TIs) realize an unconventional electronic phase originating from time-reversal symmetry and strong spin-orbit interaction (SOI). These materials are bulk insulators but possess conducting surface states in the bulk band gap. The surface states are topologically protected against non-magnetic disorder. However, impurities which break time-reversal symmetry induce a band gap in the system. This is of critical importance for potential device applications involving spin-based transport. In this work, we present a density-functional-theory study of the magnetic properties of a Fe monolayer on the (111) surface of the topological insulator Sb2Te3. We optimize the geometry of the system and determine the band structure and the easy axis of magnetization for the Fe atoms. We show that the easy axis is in-plane. In spite of this, the presence of the monolayer leads due to the opening of a gap of the order of meV, due to the interplay between magnetism and warping effects. Finally, we discuss the relevance of our findings to recent experiments about magnetic adatoms and monolayers deposited on TIs.

TT 57.9 Wed 17:15 H32

Towards topological tunnel devices - A versatile method for processing tunnel junctions from high quality single crystals — •Robin Klett[1,2], Karsten Rott[1,2], Daniel Ebke[3], Chandra Shekhar[3], Joachim Schönle[4], Wolfgang Wernsdorfer[4], Stuart Parkin[5], Claudia Felser[1,2], and Günter Reiss[1,2] — [1]Physics Department, Bielefeld University, Germany — [2]Center for Spinelectronic Materials and Devices, Universitätsstraße 25, 33605 Bielefeld, Germany — [3]Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [4]CNRS, Institut NEEL and Univ. Grenoble Alpes, F-38000 Grenoble, France — [5]Max Planck Institute for Microstructure Physics, 06120 Halle/Saale, Germany

We present a new and versatile concept for devices based on topological materials. To maintain their topological character high quality samples with clean interfaces to adjacent functional device components are mandatory. This requirement forms a bottleneck of current research, because very often the established thin film deposition fails to produce such high quality samples and bare surfaces of single crystals lack the necessary flatness. We demonstrate a novel, all-in-ultrahigh-vacuum process that enables to realize, e.g. tunnel junctions, Andreev contacts or SQUID rings from single crystalline bulk material. The validity of the technique is verified and illustrated with tunnel junctions made from cleaved single crystals of the half-Heusler topological superconductor candidate YPtBi.

TT 57.10 Wed 17:30 H32

Effective geometric phases and topological transitions in SO(3) and SU(2) rotations — •Henri Saarikoski[1], J. Enrique Vázquez-Lozano[2], José Pablo Baltanás[2], Junsaku Nitta[3], and Diego Frustaglia[2] — [1]RIKEN Center for Emergent Matter Science, Japan — [2]Departamento de Física Aplicada II, Universidad de Sevilla, Spain — [3]Department of Materials Science, Tohoku University, Japan

We address the development of geometric phases in classical and quantum magnetic moments (spin-1/2) precessing in an external magnetic field. We show that nonadiabatic dynamics lead to a topological phase transition determined by a change in the driving field topology. The transition is associated with an *effective* geometric phase which is identified from the paths of the magnetic moments in a spherical geometry. The topological transition presents close similarities between SO(3) and SU(2) cases but features differences in e.g. the limiting values of the geometric phases [1]. We discuss possible experiments where the effective geometric phase would be observable [2].
[1] H. Saarikoski, J. E. Vázquez-Lozano, J. P. Baltanás, J. Nitta, and D. Frustaglia, arXiv:1511.08315 (2015). [2] H. Saarikoski, J. E. Vázquez-Lozano, J. P. Baltanás, F. Nagasawa, J. Nitta, and D. Frustaglia, Phys. Rev. B 91, 241406(R) (2015).

TT 58: Transport: Poster Session

Time: Wednesday 15:00–18:30 Location: Poster D

TT 58.1 Wed 15:00 Poster D

Second-order coherence of microwave photons emitted by a quantum point contact — •Daniel Otten and Fabian Hassler — JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany

Shot-noise of electrons that are transmitted with probability T through a quantum point contact (biased at a voltage V_0) leads to a fluctuating current that in turn emits radiation in the microwave regime. By calculating the Fano factor F for the case where only a single channel contributes to the transport, it has been shown that the radiation produced at finite frequency ω_0 close to $eV_0/\hbar$ and at low temperatures is nonclassical with sub-Poissonian statistics ($F < 1$). It is the fermionic nature of the electrons producing the radiation, which reduces the probability of simultaneous emission of two or more photons. However, the Fano factor, being a time-averaged quantity, offers only limited information about the system. Here, we calculate the second-order coherence $g^{(2)}(\tau)$ for this source of radiation. We show that due to the interference of two contributions, two photon processes (leading to bunching) are completely absent at zero temperature for $T = 50\,\%$. At low temperatures, we find a competition of the contribution due to Gaussian current-current fluctuations (leading to bunching) with the one due to non-Gaussian fluctuations (leading to antibunching). We show that the competition of the two contributions leads to a non-monotonic behavior of the second-order coherence as a function of time so that there are times for which the second-order coherence remains below 1 at temperatures where the Fano factor is already above 1.

TT 58.2 Wed 15:00 Poster D

Energy transport in nanosystems: master equations ap-

proaches — •Kevin Marc Seja[1], Carsten Timm[1], Andreas Wacker[2], and Gediminas Kiršanskas[2] — [1]Institute of Theoretical Physics, TU Dresden, 01062 Dresden, Germany — [2]Division of Mathematical Physics, Lunds universitet, Box 118, 22100 Lund, Sweden

Master equations are a powerful tool to perform quantum-transport calculations in non-equilibrium scenarios. We use a sequential-tunneling Redfield-type approach, which includes off-diagonal elements of the reduced density matrix, to study the thermoelectric properties of nanosystems. We examine how these off-diagonal elements alter physical observables. One point of particular interest is the linear response predicted by such an approach, especially the validity of the Onsager reciprocal relations. An interacting double quantum dot serves as an exemplary system to demonstrate our main results.

TT 58.3 Wed 15:00 Poster D

Transient dynamics in electron transport through an Anderson impurity: A hierarchical quantum master equation approach — •Jakob Bätge, Sebastian Wenderoth, and Rainer Härtle — Institut für theoretische Physik, Georg-August-Universität Göttingen

We investigate the transport properties of an Anderson impurity under the influence of time-dependent electric fields. This includes the transient dynamics starting from product and correlated initial states and the response to voltage pulses, as they are used, for example, in pump-probe experiments. Our study is based on the quantum master equation methodology, where, in particular, we present an extension of the recently developed hierarchical quantum master equation approach [1] to time-dependent problems. The approach is time-local and numerically exact, as was corroborated recently for a time-independent problem by a direct comparison to quantum Monte Carlo simulations [2]. Thus, we have access to a systematic and controlled protocol to simulate long-lived correlated dynamics [3]. Here, we use this method to calculate the magnetization and the electrical current that is flowing through the impurity as a function of time, elucidating the role of resonant, non-resonant and higher-order processes.
[1] R. Härtle *et al.*, PRB **88**, 235426 (2013)
[2] R. Härtle *et al.*, PRB **92**, 085430 (2015)
[3] R. Härtle *et al.*, PRB **90**, 245426 (2014)

TT 58.4 Wed 15:00 Poster D

Zero-bias anomalies in electron transport through quantum dots for temperatures above the Kondo temperature — •Sebastian Wenderoth, Jakob Bätge, and Rainer Härtle — Institut für theoretische Physik, Georg-August-Universität Göttingen

We study the influence of exchange interactions on the steady-state transport properties of simple quantum dot structures that can be described by the single-impurity Anderson model and its spinless counterpart. To this end, we employ the quantum master equation methodolody, including a numerically exact, hierarchical technique [1,2] and, as an additional analytical tool, the Born-Markov approximation. We show that exchange interactions can lead to a zero-bias anomaly in the conductance, even for temperatures that are much higher than the respective Kondo temperature. The comparison of exact and approximate results allows us to reveal the underlying physical mechanisms, in particular the role of first- and second-order processes, decoherence and renormalization effects.
[1] R. Härtle *et al.*, PRB **88**, 235426 (2013)
[2] R. Härtle *et al.*, PRB **92**, 085430 (2015)

TT 58.5 Wed 15:00 Poster D

Andreev current through a quantum dot with spin-orbit coupling — •Daniel Spannenkrebs, Stephan Weiss, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

We study an interacting quantum dot in the presence of spin-orbit interaction. The dot is coupled to a normal and a superconducting lead. We integrate out the superconductor in the limit of an infinite gap $\Delta \to \infty$. This yields a model which consists of the normal lead and an effective dot with finite pairing amplitude. The coupling of the normal lead to the effective system is taken into account by a real-time diagrammatic method [1]. The calculation of the nonequilibrium Andreev current allows us to investigate the interplay between SO coupling and superconducting correlations on the quantum dot.
[1] M. Governale, M. G. Pala, and J. König, PRB **77**, 134513 (2008).

TT 58.6 Wed 15:00 Poster D

Thermopower signatures and spectroscopy of the canyon of conductance suppression — •Gediminas Kiršanskas, Susanna Hammarberg, Olov Karlström, and Andreas Wacker — Mathematical Physics and NanoLund, Lund University, Box 118, S-22100 Lund, Sweden

Interference effects in quantum dots between different transport channels can lead to a strong suppression of conductance, which cuts like a canyon through the common conductance plot [1]. We consider the thermoelectric transport properties of this canyon of conductance suppression using the second-order von Neumann approach. We observe a characteristic signal for the zeros of the thermopower. This demonstrates that thermoelectric measurements are an interesting complimentary tool to study complex phenomena for transport through confined systems.
[1] H. A. Nilsson et al., PRL **104**, 186804 (2010)

TT 58.7 Wed 15:00 Poster D

Interaction effects in a nanoscale heat engine — •Christian Schiegg[1], Michael Dzierzawa[1], Ulrich Eckern[1], and Karol Izydor Wysokinski[2] — [1]Institut für Physik, Universität Augsburg, Augsburg, Germany — [2]Institute of Physics, Maria Curie-Sklodowska University, 20-031 Lublin, Poland

We consider the three-terminal heat engine based on resonant tunneling through quantum dots that has been proposed by Jordan et al. [1] as an efficient energy harvester. The setup consists of a central heat reservoir coupled to a left and a right lead via resonant tunneling through tunable quantum dots that act as energy filters. Interaction effects on the performance of this heat engine have been taken into account by an effective potential that arises from the screened Coulomb interaction in the non-linear transport regime [2]. Here, we include a short-range repulsion between the leads and the quantum dots within a self-consistent Hartree-Fock approximation for the non-equilibrium steady state. The efficiency and the maximum power of the heat engine are calculated and compared with the non-interacting system and with the results obtained in [2].
[1] A.N. Jordan, B. Sothmann, R. Sanchez, and M. Büttiker, PRB **87**, 07513 (2013).
[2] B. Szukiewicz, U. Eckern, and K. I. Wysokinski, unpublished (2015).

TT 58.8 Wed 15:00 Poster D

Spin-charge coupled dynamics induced by a nonequlibrium magnetization — •Sebastian Tölle[1], Cosimo Gorini[2], and Ulrich Eckern[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Faculty of Physics, University of Regensburg, 93040 Regensburg, Germany

We discuss spin-charge coupled dynamics in a thin metallic film modelled as a two-dimensional electron gas. A proximity-induced dynamical magnetic texture, from a ferromagnet in contact with the normal metal, gives rise to an effective driving force acting on the conduction electrons. Due to the inversion asymmetry of the ferromagnet/normal metal/vacuum structure, we consider an effective Bychkov-Rashba spin-orbit interaction. We show that the latter, together with anisotropic Elliott-Yafet spin relaxation, yields important corrections to the dynamical magnetization-induced effective force. We analyze in particular the spin-pumping configuration of typical experimental setups. A non-trivial competition between the inverse spin Hall and the spin galvanic (inverse Edelstein) effects, both contributing to the build-up of a DC voltage in the sample, is found.

TT 58.9 Wed 15:00 Poster D

Spin-polarized current through the half-metallic Heusler alloy NiMnSb — •Andreas Prinz-Zwick and Rui-Jing Zhang — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Spintronics is an important field of research because of the various possible applications for such devices, for example, transistors and storage media. Heusler alloys are most interesting in this regard because of their half-metallic properties. In this context, we investigate the spin resolved transmission through the Heusler alloy NiMnSb. The calculation of the band structure of NiMnSb as well as the structural optimization were done using Density Functional Theory as implemented in the SIESTA program. The transport setup contains two semi-infinite leads of gold and a layer of NiMnSb with variable thickness in between. For the calculation of the transport properties we used the SMEAGOL program for electronic transport, which utilizes

non-equilibrium Green's functions to calculate the transmission coefficient and the Landauer formula to calculate the current. We find highly spin-polarized currents even with very thin layers of NiMnSb, for example, the spin polarization already exceeds 90% for two unit cells.

TT 58.10 Wed 15:00 Poster D

Simulation of Dipolar Quantum Magnetism with Arrays of Superconducting Qubits — •Phani Raja Muppalla — Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences & Institute for Experimental Physics, University of Innsbruck, A-6020 Innsbruck, Austria

We propose a novel platform for quantum many body simulations of dipolar XY models using state of the art circuit QED technology. Our basic building blocks are 3D Transmon qubits where we use the naturally occurring dipolar interactions to realize interacting spin systems. In order to understand the interaction of two 3D transmons for this proposal we performed numerical simulations using ANSYS HFSS. This opens the way towards the realization of a broad class of tunable spin models in both two- and one-dimensional geometries. We illustrate the possibilities on a simple XY ladder model and show how Dimer phases occurring in this model are robust against disorder and decoherence, and could be observed within state-of-the-art experiments.

[1] M. Dalmonte, S. Mirzaei, P. R. Muppalla, D. Marcos, P. Zoller, G. Kirchmair, PRB **92**, 174507 (2015)

TT 58.11 Wed 15:00 Poster D

Quantum state tomography on long-coherent superconducting transmon qubit — •Andre Schneider, Jochen Braumüller, Steffen Schlör, Martin Weides, and Alexey Ustinov — Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe

The state of a qubit is commonly measured by probing a readout resonator coupled to it with a readout tone and detecting the dispersive shift of the resonator. This measurement only gives access to the z-component of the qubit state. Quantum state tomography provides a measurement for all components of the Bloch vector by rotating the qubit state prior to the readout. We present a method of measuring the Bloch vector components. This method is demonstrated by measuring the time evolution for long-"living" transmon qubits with T_1 and T_2 times in excess of $10\,\mu$s. By recording the decay trace of the qubit state after a slightly detuned $\left(\frac{\pi}{2}\right)^x$ pulse, we detect decay and dephasing as well as Larmor precession of the qubit.

Furthermore, we introduce a benchmark for measuring the qubit manipulation fidelity and optimize the envelopes of the qubit manipulation pulses. Quantum state tomography is a powerful tool to observe changes in the qubit quantum state under interactions with magnonic systems.

TT 58.12 Wed 15:00 Poster D

Characterization of 3D-transmons and rectangular waveguides for transmission experiments — •Lukas Grünhaupt[1], Marcel Langer[1], Jochen Braumüller[1], Andre Schneider[1], Hannes Rotzinger[1], Alexander Averkin[2], Alexey V. Ustinov[1,2], and Martin Weides[1,3] — [1]Institute of Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]National University of Science and Technology MISIS, Moscow 119049, Russia — [3]Material Science in Mainz, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

We report on experiments with 3D-transmon qubits designed and fabricated at KIT. Time domain measurements of our first sample in a 3D aluminum cavity show a lifetime T1 = 1.6 μs and dephasing time T2 = 2.0 μs. By improving the cavity design, we could increase the coherence times by one order of magnitude to T1 = 16 μs and T2 = 13 μs (spin echo dephasing time T2* = 30 μs).

Our goal is to advance the 3D*concept by performing transmission experiments in a rectangular hollow core waveguide, therefore having the superconducting qubit in a truly three-dimensional environment. Consequently, we designed and fabricated a copper waveguide compatible with our cryogenic measurement setup, paying special attention to the impedance matching sections between the coaxial microwave line and the waveguide. We show preliminary transmission measurements at mK temperatures and present the challenges associated with measuring a transmon in a hollow core waveguide.

TT 58.13 Wed 15:00 Poster D

Tuning decoherence in superconducting transmon qubits by mechanical strain — •Jan Brehm, Alexander Bilmes, Georg Weiss, Alexey Ustinov, and Juergen Lisenfeld — Karlsruher Institut fuer Technologie, Karlsruhe, Deutschland

Two-level tunneling systems (TLS) are formed by structural defects in disordered materials. They gained recent attention as an important decoherence source in superconducting qubits, where they appear on surface oxides and at film interfaces. Although the most advanced qubits do not show avoided level crossings arising from a strong coupling to individual TLS, they commonly display a pronounced frequency dependence of relaxation rates, with distinguishable peaks that may point towards weak resonant coupling to single TLS [1]. Previously, we have shown that TLS are tunable via an applied mechanical strain [2]. Here, we employ this method to test whether the characteristic decoherence spectrum of a transmon qubit sample responds to changes in the applied strain, as it can be expected when the decohering bath is formed of atomic TLS. In our experiment, we will employ a highly coherent X-mon qubit sample [1] and tune the strain by bending the qubit chip via a piezo actuator. Our latest results will be presented.

[1] R. Barends et al., PRL **111**, 080502 (2013)
[2] G. J. Grabovskij et al., Science **12**, 232 (2012)

TT 58.14 Wed 15:00 Poster D

Coupling a gate tunable qubit to a 3D cavity — •Steffen Schlör[1], Patrick Zellekens[2], Thomas Schäpers[2], Alexey V. Ustinov[1], and Martin Weides[1,3] — [1]Physikalisches Institut, Karlsruhe Institut of Technology — [2]Peter Grünberg Institut (PGI9), Forschungszentrum Jülich — [3]Institute of Physics, Johannes Gutenberg University Mainz

The goal of the presented work is to implement a voltage tunable superconducting qubit. This kind of circuit could simplify architectures for quantum processors and enable the use of tunable qubits in magnetically sensitive environments. Electrostatic tunability of the Josephson coupling energy can be realized by using a superconductor/semiconductor nanowire as a weak link [1]. The field-dependent charge carrier density in the semiconductor provides a tunable nonlinear inductance.

The presented design includes a 3D microwave cavity promising good isolation of the qubit from the environment. Spectroscopy and time-resolved microwave measurements are performed in a wet ^{3}He/^{4}He cryostat at a temperature of 20 mK. We show simulations of the coupling to the cavity via the electric dipole moment as well as the electromagnetic field distribution. This coupling is important with respect to the electrostatic gate electrode, which has to be implemented without affecting the qubit coherence. Preliminary measurements of the mode spectrum show high internal coherence of the cavity.

[1] Larsen et al., PRL **115**, 127001 (2015)

TT 58.15 Wed 15:00 Poster D

Multiple transmon qubits manipulation and readout through a shared coplanar waveguide resonator — •Ping Yang[1], Jochen Braumülle[1], Andre Schneider[1], Lukas Grünhaupt[1], Lucas Radtke[1], Sebastian Skacel[1], Kirill Shulga[2], Alexey V. Ustinov[1,2], and Martin Weides[1,3] — [1]Physikalisches Institut, KIT, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Germany — [2]Russian Quantum Center, Moscow region 143025, Russia and National University of Science and Technology MISIS, Moscow 119049, Russia — [3]Materials Science in Mainz, Johannes Gutenberg-Universität Mainz, 55128 Mainz

Superconducting quantum bits (qubits) have attracted significant attention because of their applications for quantum information processing. In order to explore the scalability of superconducting qubits and their collective behavior, we investigate a quantum register formed by up to 8 transmon qubits which could all be manipulated and read out at the same time through a mutual coplanar waveguide resonator. Every qubit is designed to be tunable in frequency and has its own local bias flux. In this way, individual qubits could be either tuned into resonance with the resonator or with each other to allow information exchange, or far detuned to preserve their quantum state. Samples are designed and fabricated in our lab employing electron beam lithography and optical lithography, and then measured in the dilution refrigerator at 20 mK.

TT 58.16 Wed 15:00 Poster D

Quantum Fabry-Perot Interferometer with 3d-transmons — •Maximilian Zanner[1], Lukas Grünhaupt[1], Moritz Kappeler[1], Alexey Ustinov[1,2], and Martin Weides[1,3] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

— [2]National University of Science and Technology MISIS, Moscow 119049, Russia — [3]Material Science, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

Quantum information processing requires the ability to communicate between different parts within a specific architecture of quantum elements. In order to control the information flux the photons require a propagation channel and non-linear elements. Based on an experiment suggested by Fratini et al. [1] we are trying to build a system of two transmon qubits capacitatively coupled to a rectangular waveguide acting as a Quantum Fabry-Perot Interferometer in the single photon microwave regime. A numerical analysis shows that very unique rectification properties arise caused by the coupling between the two transmon qubits with the waveguide and each other. With the right positioning and detuning of the quantum mirrors it is possible to reach rectification factors of R > 0.92. That indicates non-reciprocal effects that were not covered in previous experiments.

[1] F. Fratini et al., PRL **113**, 243601 (2014)

TT 58.17 Wed 15:00 Poster D

Chains of nonlinear and tunable superconducting resonators — •Michael Fischer[1,2,3], Friedrich Wulschner[1,2], Peter Eder[1,2,3], Jan Goetz[1,2], Edwar Xie[1,2,3], Frank Deppe[1,2,3], Kirill Fedorov[1], Hans Hübl[1,2,3], Achim Marx[1], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

We present progress towards the fabrication and characterization 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, nonlinear and tunable superconducting resonators. The nonlinearity is achieved by galvanically coupled SQUIDs, placed in the current anti-node of each resonator and can be tuned by external coils and on-chip antennas.

This work is supported by the German Research Foundation through SFB 631 and FE 1564/1-1, EU projects CCQED, PROMISCE, the doctorate program ExQM of the Elite Network of Bavaria.

TT 58.18 Wed 15:00 Poster D

Circuit QED with 3D cavities — •Edwar Xie[1,2,3], Peter Eder[1,2,3], Michael Fischer[1,2,3], Jan Goetz[1,2,3], Max Haeberlein[1,2], Karl Friedrich Wulschner[1,2], Frank Deppe[1,2,3], Kirill 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

In typical circuit QED systems, on-chip superconducting qubits are coupled to integrated coplanar microwave resonators. Due to the planar geometry, the resonators are often a limiting factor regarding the total coherence of the system. Alternatively, similar hybrid systems can be realized using 3D microwave cavities.

Here, we present studies on transmon qubits capacitively coupled to 3D cavities. The internal quality factors of our 3D cavities, machined out of high purity aluminum, are above $1.4 \cdot 10^6$ at the single photon level and a temperature of 50 mK. For characterization of the sample, we perform dispersive shift measurements up to the third energy level of the qubit. We show simulations and data describing the effect of the transmon geometry on it's capacitive properties. In addition, we present progress towards an integrated quantum memory application.

We acknowledge support by the German Research Foundation through SFB 631 and FE 1564/1-1, the EU project PROMISCE, and Elite Network of Bavaria through the program ExQM.

TT 58.19 Wed 15:00 Poster D

Displacement of two-mode squeezed propagating microwave states — •Patrick Yard[1,2], Kirill Federov[1,2], Ling Zhong[1,2,3], Stefan Pogorzalek[1,2], Peter Eder[1,2,3], Michael Fischer[1,2,3], Jan Goetz[1,2], Friedrich Wulschner[1,2], Edwar Xie[1,2,3], Edwin Menzel[1,2], Frank Deppe[1,2,3], Achim Marx[1], and Rudolf Gross[1,2,3] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, Technische Universität München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

We study an experimental implementation of the displacement operation on squeezed microwave states. We generate these states using a conventional Josephson parametric amplifier and implement displacement using a specific cryogenic directional coupler. We demonstrate that even for strong displacement amplitudes we do not observe any degradation of the reconstructed quantum states. Furthermore, we investigate the single-mode and two-mode displacement regimes. This allows us to experimentally verify commutation relations between displacement and squeezing operators in a multi-mode case.

We acknowledge support by the German Research Foundation through SFB 631 and FE 1564/1-1, the EU project PROMISCE, and Elite Network of Bavaria through the program ExQM.

TT 58.20 Wed 15:00 Poster D

Implementation of Quantum Stochastic Walks — •Peter Schuhmacher, Luke Govia, Bruno Taketani, and Frank Wilhelm — Universität des Saarlandes

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 [1]. 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 [2]. Here, we focus on the physical realizability of both kinds of quantum stochastic walks (continuous-time and discrete-time).

[1] J. D. Whitfield, C. A. Rodríguez-Rosario and A. Aspuru-Guzik, PRA **81**, 022323 (2010).
[2] H. J. Briegel & G. De las Cuevas, Scientific Reports, 400 (2012).

TT 58.21 Wed 15:00 Poster D

Circuit QED with hybrid metamaterial transmission lines — •Stefan Ruloff, Bruno Taketani, and Frank Wilhelm — Theoretical Physics, Universität des Saarlandes, Saarbrücken, Germany

We're working on the theory of metamaterials providing some interesting results. The negative refraction index causes an opposite orientation of the wave vector **k** and the Poynting vector **S** of the travelling waves. Hence the metamaterial has a falling dispersion relation $\partial\omega(k)/\partial k < 0$ implying that low frequencies correspond to short wavelengths. Metamaterials are simulated by left-handed transmission lines consisting of discrete arrays of series capacitors and parallel inductors to ground [1]. Unusual physics arises when right-and left-handed transmission lines are coupled forming a hybrid metamaterial transmission line [2]. E.g. if a qubit is placed in front of a hybrid metamaterial transmission line terminated in an open circuit, the spontaneous emission rate is weakened or unaffected depending on the transition frequency of the qubit. Some other research interests are the general analysis of metamaterial cavities and the mode structure of hybrid metamaterial cavities for QND readout of multi-qubit operators [3]. Especially the precise answer to the question about the definition of the mode volume of a metamaterial cavity is one of our primary goals.

[1] G. Eleftheriades, A. Iyer & P. Kremer, IEEE Trans. Microw. Theory Tech. **50**, 2702 (2002)
[2] D.J. Egger and F.K. Wilhelm, PRL **111**, 163601 (2013)
[3] L. C. G. Govia et al., Phys. Rev. A **92**, 022335 (2015).

TT 58.22 Wed 15:00 Poster D

Two-qubit Quantum Gates on Qubit Chains — •Raphael Salchner[1], Daniel Egger[2], and Frank Wilhelm-Mauch[3] — [1]Universität des Saarlandes, Saarbrücken, DE — [2]Universität des Saarlandes, Saarbrücken, DE — [3]Universität des Saarlandes, Saarbrücken, DE

Quantum computers are of huge interest for scientific research and applications for their ability to solve exponentially scaling problems. There are several physical implementations of quantum bits, one of them is the superconducting qubit which is built out of Josephson junctions [1]. Usually two qubits are coupled via a resonator, but research has shown that quantum gates can be executed via direct coupling of the qubits [2]. We investigate the effect of weakly coupled idling qubits on two-qubit gate operations. We use numerical optimal control algorithms (GRAPE, Nelder-Mead Simplex) [3] to find control pulses for the Controlled-Z gate, which is important for entangling two qubits. The results indicate that already one spuriously coupled idling

qubit can cause the optimization to reach less than 99% gate fidelity, independent of the positioning of the qubits in the circuit. Additionally, several attempts are made to find control pulses that compel the desired gate, all without relevant success.

[1] D. diVincenzo, "Quantum Information Processing: Lecture Notes", 44th IFF Spring School vol. 52, FZ Jülich (2013)
[2] R. Barends et al, arXiv:1402.4848
[3] Navin Khaneja et al., J. Magn. Reson. **172**, 296 (2005)

TT 58.23 Wed 15:00 Poster D

Purcell filtering in circuit QED - Markovian and non-Markovian theory — •Dominik Schramm[1], Frank Wilhelm[1], and Karl-Peter Marzlin[2] — [1]Universität des Saarlandes, 66123 Saarbrücken, Germany — [2]Department of Physics, St. Francis Xavier University, Antigonish, Nova Scotia, B2G 2W5, Canada

In circuit QED the measurement fidelity is limited by the Purcell effect, which means a decay of the qubit state through the resonator into the transmission line. This energy leakage can be suppressed by using a bandpass Purcell filter. We study decoherence effects of a system with a Purcell filter by deriving a master equation for the reduced density matrix. We look at the crossover between resonant and dispersive regime. We study in particular the non-Markovian regime to compare the Purcell filter to other suppression methods.

TT 58.24 Wed 15:00 Poster D

Interacting two-level defects as sources of fluctuating high-frequency noise in superconducting circuits — •Clemens Müller[1], Jürgen Lisenfeld[2], Alexander Shnirman[3,4], and Stefano Poletto[5] — [1]ARC Centre of Excellence for Engineered Quantum Systems, The University of Queensland, Brisbane, Austrlalia — [2]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Institut für Theory der Kondensierten Materie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [4]LD Landau Institute for Theoretical Physics, Moscow, Russia — [5]IBM TJ Watson Research Centre, Yorktown Heights, USA

Since the very first experiments, superconducting circuits have suffered from strong coupling to environmental noise, destroying quantum coherence and degrading performance. In state-of-the-art experiments, it is found that the relaxation time of superconducting qubits fluctuates as a function of time. We present measurements of such fluctuations in a 3D-transmon circuit and develop a qualitative model based on interactions within a bath of background two-level systems (TLS) which emerge from defects in the device material. In our model, the time-dependent noise density acting on the qubit emerges from its near-resonant coupling to high-frequency TLS which experience energy fluctuations due to their interaction with thermally fluctuating TLS at low frequencies. We support the model by providing experimental evidence of such energy fluctuations observed in a single TLS in a phase qubit circuit.

TT 58.25 Wed 15:00 Poster D

Decoherence dynamics in a finite-size quantum Ising model. — •Cyril Saussol, Wolfgang Belzig, and Gianluca Rastelli — University of Konstanz Fachbereich Physik D-78457, Konstanz, Germany.

We study the non-equilibrium dynamics of a quantum Ising chain with N spins coupled to a bath. We consider as initial state an entangled state formed by two many-spin classical states. In the limit in which the transversal magnetic field (TMF) vanishes, the system contains a decoherence-free subspace (DFS). Moreover, this model has also an exact solution. Hence we tackle the problem by using a perturbative approach in the TMF to study the decoherence dynamics. In particular, we are interested to calculate analytically the decoherence time if the system is initialized in an entangled state of the DFS. Finally, we discuss the perspectives of how to prepare optimal, initial entangled states (formed by more than two classical states) in order to increase the decoherence time.

TT 58.26 Wed 15:00 Poster D

Proximity effect in normal-superconductor hybrids for quasiparticle traps — •Amin Hosseinkhani — Peter Grunberg Institute (PGI-2), Forschungszentrum Julich, D-52425 Julich, Germany — JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany

Coherent transport of charges in the form of Cooper pairs is the main feature of Josephson junctions which plays a central role in superconducting qubits. However, the presence of quasiparticles in superconducting devices may lead to incoherent charge transfer and limit the coherence time of superconducting qubits. A way around this so-called "quasiparticle poisoning" might be using a normal-metal island to trap quasiparticles; this has motivated us to revisit the proximity effect in normal-superconductor hybrids. Using the semiclassical Usadel equations, we study the density of states (DoS) both within and away from the trap. We find that in the superconducting layer the DoS quickly approaches the BCS form; this indicates that normal-metal traps should be effective at localizing quasiparticles.

TT 58.27 Wed 15:00 Poster D

shot noise of 1,4-benzenedithiol single-molecule junctions — •Amin Karimi[1], Safa Golrokh[1], Markus Herz[1], Ryoma Hayakawa[1,2], Fabian Pauly[1], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, Konstanz, Germany — [2]Advanced Electronic Materials Center, National Institute for Materials Science, Namiki, Tsukuba, Japan

Shot noise measurements represent an important tool to characterize quantum transport through nanoscale junctions [1,2]. However, noise measurements are difficult since extrinsic noise sources have to be carefully discarded from the intrinsic signal. We present here a much simpler experimental technique compared to established methods that is operational over several orders of magnitude of conductance and noise. It does not impose additional requirements on the measurement wiring and uses solely commercially available electronics. The performance of the system is tested by investigation of established gold single-atom contacts. We then apply the novel method to single-molecule contacts of benzenedithiol (BDT) between Au electrodes. Our study hence reports that Au-BDT-Au is a molecular junction with a widely tunable conductance. It represents the conceptually simplest quantum system, namely a single channel, quantum coherent junction.

[1] D.Djukic, J. M. van Ruitenbeek, Nano Lett. **6**, 789 (2006)
[2] O. Tal, M. Krieger, B. Leerink, J. M. van Ruitenbeek, PRL **100**, 196804 (2008)

TT 58.28 Wed 15:00 Poster D

Time-dependent transport in molecular junctions using hierarchical quantum master equations — •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

Time-dependent currents in molecular junctions can be caused by structural fluctuations or interaction with external fields. In this contribution, we demonstrate how the hierarchical quantum master equation approach can be used to study time-dependent transport in a molecular junction. This reduced density matrix methodology provides an accurate solution to the transport problem including time-dependent energy levels, molecule-lead coupling strengths and transitions between electronic states of the molecular bridge. Employing representative models, the influence of such time-dependencies on the electronic current is analyzed in some detail.

TT 58.29 Wed 15:00 Poster D

Conductance through a ferrocene based molecule — Karthiga Kanthsamy[1], •Ejvind Olsen[1], David Zsolt Manrique[3], Qusiy Al Galiby[3], Christoph Tegenkamp[1,2], Colin Lambert[3], and Herbert Pfnür[1,2] — [1]Institute für Festkörperphysik, Leibniz University Hannover, Hannover, Germany — [2]Laboratory for Nano and Quantum Engineering, Leibniz University Hannover, Hannover, Germany — [3]Department of Physics, Lancaster University, Lancaster LA 14YB, United Kingdom

We investigate the electrical transport through 1,1'-bis [4-thio acetyl phenyl] ferrocene (FBPDT) molecule using mechanically controllable break junction technique (MCBJ). The junctions were broken in vacuum. Two types of measurements were done. First, conductance were measured at constant voltage by repeated opening and closing of the junction. Step-wise change in conductance values are observed below 1G0 after molecular adsorption. The histogram shows dominant peaks at 0.017G0 and 0.002G0. Second, the IV characteristics were measured at stable conductance values below 1G0 which remain linear, but conductance decreases with increasing distance between the electrodes. The theoretical calculations based on density functional theory and non-equilibrium Green's function formalism shows that the rotation of the phenyl ring influences the transmission through the molecule. The

molecule is energetically degenerate irrespective of rotation of phenyl ring angle with respect to the cyclo pentyl ring. The phenyl rings act as tunneling barriers resulting in lower conductance compared to ferrocene dithiol.

TT 58.30 Wed 15:00 Poster D

Improved auxiliary-mode approach to time-dependent electron transport — •Bogdan Popescu and Alexander Croy — Max Planck Institut for the Physics of Complex Systems

The theoretical description of time-resolved phenomena in nanoscale devices remains a very challenging task. Several formalisms are available, but efficient approaches for general-purpose computations are still under investigation. In [1] it was proposed to use an auxiliary-mode expansion of the self-energies arising in the time-dependent non-equilibrium Greens function (TDNEGF) formalism. To this end the Fermi function and the level-width function are expanded in terms of simple poles (Lorentzians). This procedure converts the integro-differential equation for the reduced density-matrix into a set of coupled differential equations for auxiliary matrices.

In this contribution we present an improved version of the auxiliary-mode approach, where the auxiliary matrices are replaced by vectors or scalars. This drastically reduces the computational effort and memory requirement of the method. We demonstrate the method using a molecular wire and graphene nanoribbons as examples.

[1] A. Croy and U. Saalmann, PRB **80**, 245311 (2009)

TT 58.31 Wed 15:00 Poster D

Resistance study of the unusual metal-insulator-transition in the organic charge-transfer salt κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl — •C. Delleske[1], D. Zielke[1], E. Gati[1], H. Schubert[1], J.A. Schlueter[2], and M. Lang[1] — [1]Physikalisches Institut, SFB TR 49, Goethe Universität, 60438 Frankfurt, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA

Materials close to a correlation-driven metal-insulator transition are known to show a variety of intriguing phenomena such as anomalous metallic and superconducting states. The organic charge-transfer salts of the BEDT-TTF family provide an ideal playground for studying the interplay between metallic and insulating phases, because of the simultaneous action of on-site and inter-site Coulomb repulsion and their low-dimensionality. Recently, κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl has attracted particular interest since it shows a metal-insulator transition at $T_{MI} = 30\,\mathrm{K}$ which has been assigned to charge order [1] , in combination with very strong frustration ($t'/t = 0.84$) [2]. In this contribution, we investigate the in-plane resistivity of crystals which have been grown in our own laboratory. We show that the resistivity jump at the transition is as high as reported in literature [3] indicating comparable high quality of our crystals. A significant hysteresis at the phase transition can be observed in contrast to literature results [3]. Furthermore, we discuss anomalous hysteresis effects in the metallic state.

[1] N. Drichko et al., PRB **89**, 075133 (2014)
[2] H. Jeschke, private communication
[3] S. Yasin et al., Physica B **407**, 1689 (2012).

TT 58.32 Wed 15:00 Poster D

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. Conducting layers of ET molecules are separated by thin, insulating anion layers X, resulting in a quasi-2D electronic band structure. The ET 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 exhibits a gap in the charge-carrying excitations caused by the Coulomb interaction between the electrons and shows antiferromagnetic ordering at $T_N \approx 27\,K$. Recently, it has been shown that disorder induced by X-ray irradiation drives the Mott insulating state with long-ranged antiferromagnetic order into a quantum spin liquid state [1]. We perform comparative measurements of fluctuation (noise) spectroscopy on pristine and irradiated (disordered) 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.

[1] T. Furukawa et al., PRL **115**, 077001 (2015).
[2] B. Hartmann et al., PRL **114**, 216403 (2015).

TT 58.33 Wed 15:00 Poster D

Transport and thermodynamic studies of the unusual metal-insulator transition in κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl under He-gas pressure — •D. Zielke[1], E. Gati[1], S. Köhler[1], S. Winter[1], H. Schubert[1], P. Lunkenheimer[2], J. A. Schlueter[3], and M. Lang[1] — [1]Institute of Physics, SFB/TR49, Goethe-University, Frankfurt, Germany — [2]University of Augsburg, Center for Electronic Correlations & Magnetism, SFB/TR80, Germany — [3]Materials Science Division, Argonne National Laboratory, USA

Organic charge-transfer salts of the BEDT-TTF family show a wide variety of electronic phases resulting from the interplay of strong on-site and inter-site Coulomb repulsion along with low dimensions. The quasi-2D κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl is distinct by a high degree of frustration of $t'/t = 0.84$ (at 50 K) [1] and reveals an unusual metal-insulator transition at $T_{\mathrm{MI}} = 30\,\mathrm{K}$ which has been associated with charge-order [2]. We present a study of dc resistance measurements at ambient and at finite hydrostatic He-gas pressure. We find that the MI transition can be rapidly shifted towards lower temperatures with increasing pressure. At $P = 97\,\mathrm{MPa}$ the system remains metallic down to 2.4 K. In addition, our results of thermal expansion measurement show discontinuous changes of the lattice parameters at T_{MI} accompanied by hysteresis which prove the 1$^{\mathrm{st}}$-order character of this transition, in contrast to literature results [3]. Moreover, we observe a glass-like transition at $T_{\mathrm{g}} \approx$ 60-65 K which is consistent with recent calculations [4].

[1] H. Jeschke, priv. comm.
[2] N. Drichko *et al.*, PRB **89**, 075133 (2014).
[3] S. Yasin *et al.*, Physica B **407**, 1689 (2012).
[4] Müller *et al.*, NJP **17**, 083057 (2015).

TT 58.34 Wed 15:00 Poster D

Origin of the Glasslike Dynamics in Molecular Conductors κ-(BEDT-TTF)$_2$X — •Benedikt Hartmann[1], Robert Rommel[1], Jens Brandenburg[1], Steve M. Winter[1], John Schlueter[2], Takahiko Sasaki[3], and Jens Müller[1] — [1]Institute of Physics, Goethe-University Frankfurt, Frankfurt (M), Germany — [2]Argonne National Laboratory, Materials Science Division, Argonne (IL), USA — [3]Institute for Materials Research, Tohoku University, Sendai, Japan

The organic molecular conductors κ-(BEDT-TTF)$_2$X exhibit a structural glasslike transition, which can be utilized (i) to modify the correlation strength of the charge carriers close to the Mott metal insulator transition [1], as well as (ii) to study the influence of intrinsic molecular disorder [2]. A deeper microscopic understanding, however, has been lacking. In this contribution we demonstrate that fluctuation (noise) spectroscopy is an effective technique to access the intrinsic properties of the glasslike transition [3]. The temperature dependence of 1/f-type fluctuations can be described by a Vogel-Fulcher-Tamman law, allowing to classify the κ-(BEDT-TTF)$_2$X-salts as highly fragile orientational glasses. Heat pulse experiments and supporting ab initio calculations provide an explanation for the origin of the observed glassy dynamics in κ-(BEDT-TTF)$_2$X in terms of a simple two-level model, making quantitative statements possible and predictions for the occurrence of glassiness in different κ-(BEDT-TTF)$_2$X systems feasible [3].

[1] B. Hartmann et al., PRL **114**, 216403
[2] B. Hartmann et al., PRB **90**, 195150
[3] J. Müller et al., NJP **17**, 083057

TT 58.35 Wed 15:00 Poster D

Inplane anisotropy of the critical field of α-(BEDT-TTF)$_2$MHg(SCN)$_4$ (M = K, Tl) — •Michael Kunz[1,2], Luzia Höhlein[1,2], Sebastian Jakob[1,2], Werner Biberacher[1], Harald Müller[3], Natalya Kushch[4], and Mark Kartsovnik[1] — [1]Walther-Meißner-Institut, Garching, Deutschland — [2]Technische Universität München, Garching, Deutschland — [3]European Synchrotron Radiation Facility, Grenoble, France — [4]Institute of Problems of Chemical Physics, Chernogolovka, Russia

The quasi-two-dimensional organic metals α-(BEDT-TTF)$_2$MHg(SCN)$_4$ (M = K, Tl) undergo a transition into a charge-density-wave (CDW) state with a transition temperature of $T_{\mathrm{CDW}} \approx 8.5\,\mathrm{K}$ for the K-compound and $T_{\mathrm{CDW}} \approx 10\,\mathrm{K}$ for the Tl-compound. At even lower temperatures an inhomogeneous superconducting (SC) state emerges with an onset temperature between 0.3 and 0.5 K. By applying pressure

the CDW state can be completely suppressed, giving way to a homogeneous bulk SC state with a sharp transition. We present the azimuthal anisotropy of the upper critical field of α-(BEDT-TTF)$_2$MHg(SCN)$_4$ (M = K, Tl) studied at different pressures above and below the critical pressure where the CDW state is fully suppressed. The experimental results are analyzed in relation to multiple band contributions to SC pairing and possible manifestations of exotic superconductivity.

TT 58.36 Wed 15:00 Poster D

Stamp transfer of carbon nanotubes for nano-electromechanics — Dominik Berndt, Patrick Steger, Julian Heger, Karl Götz, Korbinian Mühlberger, Nicola Paradiso, Christoph Strunk, and •Andreas K. Hüttel — Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

Growing "ultraclean" carbon nanotubes via chemical vapour deposition (CVD) over pre-existing contact structures involves high temperatures ($\sim 900°$C) and aggressive gases (CH_4 and H_2). Consequently this procedure imposes many limitations on the choice of the contact material, in particular regarding superconductors. Many metal thin films are either destroyed during the CVD-process or lose superconducting properties. The alternative explored here is to grow the carbon nanotubes on a separate chip and mechanically transfer them to the Si/SiO_2 chip with contact electrodes. We use a stamping procedure, growing nanotubes on a transparent SiO_2 substrate which is subsequently pressed onto the electrode chip. There the nanotubes are suspended over superconducting Nb contacts with a thickness of 100nm, separated by a 500nm wide trench. In low temperature transport, we examine gate dependence of the conductance, influences of the superconducting contacts, and mechanical features of the transferred nanotubes. The transfer method can be used for all those applications requiring materials that would not withstand the CVD growth conditions.

TT 58.37 Wed 15:00 Poster D

Magnetic field induced electron-vibron coupling in a carbon nanotube quantum dot — •Peter Stiller, Daniel Schmid, Christoph Strunk, and Andreas Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Quantum dots defined in suspended single wall carbon nanotubes define a nano-electromechanical system where clear quantized harmonic oscillator behaviour becomes visible. We present transport measurements on a clean nanotube device tuned to the few electron regime, i.e., having a highly localized electronic system. Here, we demonstrate the emergence of Franck-Condon sidebands in single electron tunneling, corresponding to the longitudinal vibration, induced by a finite magnetic field along the carbon nanotube axis. The Franck-Condon coupling factor g increases with magnetic field and saturates at $B \approx 5$ T. The behaviour of the sidebands attached to different electronic quantum states is compared, and tentative models are discussed.

TT 58.38 Wed 15:00 Poster D

Current flow paths in bent and deformed carbon nanotubes — •Eric Kleinherbers[1], Thomas Stegmann[1,2], and Nikodem Szpak[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [2]Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca

Due to imminent applications in nanoelectronics it is of high interest to understand the precise conductance properties of bent or deformed carbon nanotubes. Since low-energy electronic excitations in graphene behave like massless Dirac fermions the current flow can be approximated semiclassically and used as a guide in the design of conducting nanotube-elements. 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 58.39 Wed 15:00 Poster D

Magnetic field-effect transistor in carbon nanotubes — •Magdulin Dwedari[1], Thomas Stegmann[1,2], and Nikodem Szpak[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [2]Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca

It is well known that low-energy electronic excitations in graphene behave like massless Dirac fermions. Since particles (excitations) and antiparticles (holes) react oppositely to the magnetic field a magnetic field-effect transistor emerges when a carbon nanotube is placed in a perpendicular magnetic field and contacted appropriately. We calculate the current flow theoretically within a semiclassical model and simulate it numerically.

TT 58.40 Wed 15:00 Poster D

Gap engineering in strained carbon nanotubes with parallel magnetic field — •Lennart Korsten[1], Thomas Stegmann[1,2], and Nikodem Szpak[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [2]Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca

Strain and curvature in carbon nanotubes influence the distances and angles between the atomic orbitals. In the tight-binding description of electronic excitations, this leads to anisotropic tunneling amplitudes and to the shift of Dirac points in the energy dispersion relation. Since application of a parallel magnetic field can also move the Dirac points it can be used for opening or closing the energy gap as well as for precise measurements of the strain and curvature effects. We calculate these effects theoretically and simulate the electronic transmission numerically.

TT 58.41 Wed 15:00 Poster D

Current flow paths in deformed graphene: pseudo-magnetic field vs curvature — •Nikodem Szpak[1] and Thomas Stegmann[1,2] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [2]nstituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca

We compare two fundamentally different approaches to the electronic transport in deformed graphene: a) current flow paths obtained with the non-equillibrium Green's function (NEGF) method from the tight-binding model with local strain, b) classical trajectories for relativistic point particles moving in a curved surface with pseudo-magnetic field. The connection between them is established in the long-wave limit via an effective Dirac Hamiltonian in curved space. Geometrical optics approximation applied to focused current beams allows to directly compare the wave and the particle pictures. We obtain very good numerical agreement between the quantum and the semiclassical approaches for a fairly wide set of parameters. We propose a new mechanism of geometric lensing of currents which can find applications in nanoelectronics.

TT 58.42 Wed 15:00 Poster D

Landau quantized Dirac electrons in a photon cavity — •Lisa Hesse and Klaus Richter — Universität Regensburg, Institut für Theoretische Physik, 93040 Regensburg, Germany

We consider Landau quantized monolayer graphene exposed to an electromagnetic cavity mode. Due to the large degeneracy and Dirac-type characteristics of the Landau-level spectrum graphene is meant to show collective excitation effects under the influence of the additional radiation field in a resonant strong light-matter-coupling regime [1]. The controversially discussed [1, 2, 3] question about the existence of such Dicke-type superradiant quantum phases and connected phenomena due to photon-induced cyclotron transitions opens a challenging subfield of research in graphene. On the basis of a realistic tight-binding simulation we study the interaction of resonant cavity photon modes with Landau quantized states in graphene focusing on the spectral properties of this hybrid system.

[1] D. Hagenmüller and C. Ciuti, PRL **109**, 267403 (2012)
[2] L. Chirolli, M. Polini, V. Giovannetti and A. H. MacDonald, PRL **109**, 267404 (2012)
[3] F. M. D. Pellegrino, L. Chirolli, R. Fazio, V. Giovannetti and M. Polini, PRB **89**, 165406 (2014)

TT 58.43 Wed 15:00 Poster D

Spin-Transport in Graphene with Agregated Hydrogen Clusters — •Fedor Tkatschenko, Jan Bundesmann, Denis Kochan, Jaroslav Fabian, and Klaus Richter — Institut für Theoretische Physik Universität Regensburg

Hydrogen on graphene acts as resonant impurity and in addition can lead to formation of local magnetic moments. Both effects reduce the spin lifetime by orders of magnitude [1]. This can explain the discrepancy between predicted long spin lifetimes compared to the short ones measured in experiments. However, some experiments report a longer spin lifetime after increasing the H concentration [2].

We argue that above some threshold concentration the probability

for formation of H-clusters like dimers or trimers strongly increases. The collective impact from H-clusters can differ from isolated H-atoms. This is reflected in the systems electronic structure. Using a single-orbital tight binding approach we calculate the electronic structure for H-clusters on graphene which is shown to be in good agreement with DFT calculations. Furthermore we perform quantum transport calculations and extract the influence on the spin lifetime. We find that the exact configuration of the clusters like the sublattice occupation is essential, as it decides whether magnetic moments are formed or the position of the resonant state.

[1] D. Kochan, M. Gmitra and J. Fabian, PRL **112**, 116602 (2014)
[2] M. Wojtaszeck, I. J. Vera-Marun, T. Massen and B. J. van Wees, PRB **87**, 081402(R) (2013)

TT 58.44 Wed 15:00 Poster D

Spin and Charge Transport in Tailored Carbon Allotropes such as Doped Graphene — •Marie-Luise Braatz[1,2], Nils Richter[1,2], Markus Rein[1], Nils-Eike Weber[3], Khaled Parvez[3], Xinlian Feng[4], Hermann Sachdev[5], Klaus Müllen[5], and Mathias Kläui[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz (MAINZ), 55128 Mainz, Germany — [3]BASF SE, 67056 Ludwigshafen, Germany — [4]Molecular Functional Materials, Dresden University of Technology, 01069 Dresden, Germany — [5]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

Graphene exhibits extraordinary properties, however, pristine graphene does not have 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 varied to achieve different dopant concentrations and the ensuing materials are systematically characterized. Raman spectroscopy is employed to determine the structural effects of doping and transmission electron microscopy (TEM) can reveal the spatial distribution of dopants. Magnetoresistance effects and magnetization are probed to understand the correlation between the structural and magnetotransport properties [2]. By modifying its growth conditions, the electronic, magnetic and structural properties of graphene can thus be tuned.

[1] H. Wang et al., ACS Catal. **2**, 781 (2012).
[2] M. Rein et al., ACS Nano **9**, 1360 (2015).

TT 58.45 Wed 15:00 Poster D

Magnetotransport in Graphene on the Nano Scale — Philip Willke, •Thomas Kotzott, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Magnetotransport in graphene gives rise to a variety of fascinating phenomena like the quantum Hall effect and weak and/or strong localization. Often the origin of these phenomena lies on the atomic scale governed by the crystal structure as well as the scattering mechanisms involved. While macroscopic transport measurements only give an average over all scattering contributions, we combine magnetotransport experiments with atomic scale resolution. We introduce a new magnetic field scanning tunneling potentiometry setup to investigate the local voltage drop in epitaxial graphene below the quantum limit. While monolayer and bilayer graphene sheets show a locally varying quadratic magnetoresistance larger than the macroscopic average, scattering processes at localized defects are almost independent of magnetic field.

TT 58.46 Wed 15:00 Poster D

Pressure tuning of the electrical transport properties of the Weyl semimetal NbP — •Ricardo dos Reis, M. O. Ajeesh, Yan Sun, Chandra Shekhar, Marcus Schmidt, Claudia Felser, Binghai Yan, and Michael Nicklas — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Recently enormous attention has been given to a class of material called Weyl semimetal (WSM) due to the prediction of many exotic phenomena, in particular exceptional transport properties, making these systems not only interesting for fundamental research, but also promising materials for novel applications. WSM can be viewed as the hybrid of 3D graphene and topological insulators. The band crossing point, the so-called Weyl point, acts as a magnetic monopole (a singular point of Berry curvature) in momentum space, which always comes in a pairs. If the time-reversal and inversion symmetries are respected, a pair of Weyl points is degenerate in energy, forming another topological phase called Dirac semimetal. Owing this complex band structure the details of the electronic structure can play a significant role in the electrical transport properties of these materials. In this context, external pressure is an important control parameter to effectively tune lattice structures and the corresponding electronic states in a systematic fashion, avoiding the complexity brought by chemical doping. Here, we present a high pressure study of the magnetotransport properties of the Weyl semimetal NbP, which are particularly important to explore novel phenomena and understand the physics behind.

TT 58.47 Wed 15:00 Poster D

Magnetotransport in 3d topological insulator nanowires — •Raphael Kozlovsky, Sven Essert, Cosimo Gorini, Matthias Stosiek, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We investigate the transport characteristics of nanowires and nanotubes in external electric and magnetic fields, using mainly numerical tools. In particular, we are interested in systems consisting of three-dimensional topological insulator (3d TI) materials, which we model by bulk and surface Hamiltonians. In such 3d-TI nanowires, a magnetic field along the wire leads to prominent Aharonov-Bohm oscillations that indicate the surface nature of the Dirac states forming due to a non-trivial topological invariant. We investigate their transport properties with specific focus on wires with a non-constant radius along the wire direction giving rise to a spatial variation of the enclosed magnetic flux.

TT 58.48 Wed 15:00 Poster D

Superconductivity in Dirac semimetals — •Tatsuki Hashimoto[1], Shingo Kobayashi[1], and Masatoshi Sato[2] — [1]Nagoya university, Nagoya, Japan — [2]Kyoto university, Kyoto, Japan

In this presentation, we would like to discuss the superconductivity in Dirac semimetals. Dirac semimetal is a material that hosts topologically protected bulk Dirac cones and surface Fermi loop. It has been revealed that the unique spin-orbit interaction in the Dirac semimetals stabilize the unconventional superconductivity. Experimentally, the zero-bias conductance peak that suggests the realization of topological superconductivity has been observed in Cd_3As_2.

We use a $k \cdot p$ Hamiltonian around Γ point with spin and orbital degrees of freedom to describe the Dirac semimetal. For the model, we propose six types of k-independent pair potentials, where two of them are trivial pairings and others are topological ones. By introducing a single band description of the pair potentials, it is found that the superconducting gap and d-vector have the characteristic structure in each pair potential. To see these, we calculate the electronic specific heat and spin susceptibility and confirm that we can distinguish these superconducting states experimentally. In addition to the bulk physical properties, we also calculate the surface state by using the recursive Green's function method. It is find that either arc or flat shape Andreev bound states appear on the surface depending on the parity of mirror reflection symmetry.

TT 58.49 Wed 15:00 Poster D

Transport and Pairing properties of Helical Edges with Proximity induced Superconductivity and Ferromagnetism — •Felix Keidel[1], François Crépin[2], Pablo Burset[1], and Björn Trauzettel[1] — [1]Institute of Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [2]Laboratoire de Physique Théorique de la Matière Condensée, UPMC, Sorbonne Universités, 75252 Paris, France

The scientific interest in Quantum Spin Hall systems is far from declining. While these certainly are fascinating by themselves, there is plenty of new and exciting physics to arise when superconductivity and ferromagnetism are brought into the game. The strong constraint of helicity in the edge states of a two-dimensional topological insulator is responsible for an intimate relation between the allowed scattering processes in a hybrid junction and the parameters of the system, namely the superconducting order parameter and the magnetic field. In our work, we study a helical liquid in proximity to a conventional s-wave superconductor and ferromagnetic insulators by means of a Green's function analysis. The ferromagnet gives rise to sub-gap Andreev/Majorana bound states and non-local crossed Andreev reflection (CAR), both of which decisively affect the pairing and transport properties of the junction. As a result, the simple s-wave symmetry of the superconductor is enrichened and unconventional odd-frequency triplet superconductivity emerges. Strikingly, we have identified a setup that favors CAR over electron co-tunneling and may allow for the indirect measurement of the symmetries of the superconducting order parameter.

TT 58.50 Wed 15:00 Poster D

Optical Measurement of Carrier Mobilities in the Topological Insulator $BiSbTeSe_2$ — •Henning Kuhn, Jingyi Zhu, Matteo Montagnese, Zhiwei Wang, Yoichi Ando, and Paul H.M. van Loosdrecht — 2.Physikalisches Institut, Universität zu Köln

Transient Grating Spectroscopy, an ultrafast pump-probe technique, is employed to investigate the non-equilibrium transport properties of the topological insulator (TI) $BiSbTeSe_2$.

An optically generated periodic modulation pattern of electronic excitations is created at the surface of the TI and its decay is observed, both through the use of 100fs pulses from a mode locked Ti:Sapphire laser system. Experiments are performed in the temperature range from 10K to 300K using a heterodyne detection scheme, which, among other, show clear coherent phonon excitations. From the transient grating decay times, carrier diffusivities and thus carrier mobilities are extracted. The obtained temperature dependence of the mobility will be discussed in terms of the recently proposed puddle model, paying special attention to a potential contribution from surface carriers.

TT 58.51 Wed 15:00 Poster D

Fano Resonances in Majorana Bound State - Quantum Dot Systems — •Alexander Schuray, Luzie Weithofer, and Patrik Recher — TU Braunschweig, Institute for Mathematical Physics, Braunschweig

Majorana bound states (MBS) have recieved a lot of attention in the last years and first experiments with nanowires in proximity to a superconductor [1] possibly present first experimental evidence for their existence.

Systems in which MBS are coupled via a quantum dot to normal leads are also gaining interest, as the parameters of the dot provide an interesting handle for transport signatures [2]. In contrast to previous studies, here we consider two MBS with non-zero overlap coupled to a lead on one side and a quantum dot on the other side. Using the Keldysh formalism we derive the cumulant generating function (CGF) for the tunnel currents in the leads [3]. We show that this setup exhibits a Fano-resonance which we interpret as resulting from interference of two different transport channels. Finally, we validate numerically that our result for this simple model is also applicable to a realistic setup of quantum wire and dot.

[1] V. Mourik et al., Science **336**, 1003 (2012).
[2] G.-Y. Huang, M. Leijnse, K. Flensberg, H. Q. Xu, PRB **90**, 214507 (2014)
[3] L. Weithofer, P. Recher, T. L. Schmidt, PRB **90**, 205416 (2014)

TT 58.52 Wed 15:00 Poster D

Full Counting Statistics of Chiral Majorana Fermions — Alexander Schuray, •Luzie Weithofer, and Patrik Recher — TU Braunschweig, Institute for Mathematical Physics, Braunschweig

In recent years many detection schemes for chiral Majorana fermions interferometers [1] in which the current or noise is used to identify the Majorana character of the propagating edge states have been proposed. Here, we derive a general formalism to find the general transport properties for chiral Majorana fermions coupled to normal leads. For this we employ Full Counting Statistics [2-3], a Keldysh-technique based method, to find the so-called cumulant generating function (CGF), an expression that gives an insight into the elementary transport processes and from which the full statistics of the current can be obtained by differentiation. Our method reproduces the known results of different interferometers, like Fabry Perot [4] or Hanbury Brown-Twiss [5] in a concise way. Finally, we apply it to a three-terminal setup and discuss its transport properties.

[1] J. Li, G. Fleury, and M. Büttiker, PRB **85**, 125440 (2012).
[2] Y. Nazarov and M. Kindermann, Eur. Phys. J. B **35**, 413 (2003).
[3] L. S. Levitov and M. Reznikov, PRB **70**, 115305 (2004).
[4] K. Law, P. Lee, and T. Ng, PRL **103**, 237001 (2009).
[5] G. Strübi, W. Belzig, M.-S. Choi, and C. Bruder, PRL **107**, 136403 (2011)

TT 58.53 Wed 15:00 Poster D

Influence of Andreev tunneling on the full counting statistics — •Philipp Stegmann and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

We theoretically discuss the influence of Andreev tunneling on the full counting statistics of charge transfer. The slightest presence of Andreev tunneling yields qualitative different generalized factorial cumulants [1] for the short-time limit in comparison to the nonsuperconducting case. We illustrate this behavior for a superconducting lead weakly tunnel coupled to a normal-state metallic island [2]. By means of this example system, we demonstrate that generalized factorial cumulants can detect the presence of Andreev tunneling for longer times as well if the dependence on the parameter s or the visibly of interactions [1, 3, 4] is studied.

[1] P. Stegmann, B. Sothmann, A. Hucht, J. König, PRB **92**, 155413 (2015).
[2] V. F. Maisi, D. Kambly, C. Flindt, J. P. Pekola, PRL **112**, 036801 (2014).
[3] D. Kambly, C. Flindt, M. Büttiker, PRB **83**, 075432 (2011).
[4] D. Kambly and C. Flindt, J. Comput. Electron. **12**, 331 (2013).

TT 58.54 Wed 15:00 Poster D

Effect of the electromagnetic environment on ac driven tunnel junctions — •Moritz Frey and Hermann Grabert — Physikalisches Institut, Universität Freiburg

We analyze the effect of the lead impedance on a tunnel junction driven by a time-dependent voltage source. The external drive excites the modes of the electromagnetic environment and modifies the dynamical Coulomb blockade effect familiar from dc driven junctions. In particular, we consider the electrical current flowing in the leads of the junction when it is driven by a superposition of a constant and a sinusoidal voltage source. The electromagnetic environment gives rise to a suppression of higher harmonics of the average current. We also investigate the current noise and the validity of fluctuation-dissipation relations. Specific predictions are made for a tunnel junction driven through an LC-circuit as studied recently experimentally [1,2].

[1] C. Altimiras et al., PRL **112**, 236803 (2014)
[2] O. Parlavecchio et al., PRL **114**, 126801 (2015)].

TT 59: Low-Dimensional Systems: Poster Session

Time: Wednesday 15:00–18:30 Location: Poster D

TT 59.1 Wed 15:00 Poster D

Finite-size effects in spin-gapped metals — •Jonas Greitemann[1,3], Stephan Hesselmann[1], Stefan Wessel[1], Fakher Assaad[2], and Martin Hohenadler[2] — [1]RWTH Aachen, Germany — [2]University of Würzburg, Germany — [3]LMU Munich, Germany

Attractive backscattering in one-dimensional models is a relevant perturbation to the Tomonaga-Luttinger fixed point, prompting the opening of a spin gap as governed by the Luther-Emery fixed point. We use complementary quantum Monte Carlo approaches to show that this crossover takes place as a function of distance, giving rise to finite-size effects below a scale set by the inverse spin gap. In particular, the finite-size scaling of the staggered charge susceptibility is argued to be unreliable for pinpointing the Peierls transition in the spinful Holstein model.

TT 59.2 Wed 15:00 Poster D

Charge and spin density in the helical Luttinger liquid — Niccolò Traverso Ziani[1], •Christoph Fleckenstein[1], Francois Crépin[2], and Björn Trauzettel[3] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [2]Laboratoire de Physique Théorique de la Matière Condensée, UPMC, CNRS UMR 7600, Sorbonne Universités, 4 place Jussieu, 75252 Paris Cedex 05, France — [3]Department of Physics, University of California, Berkeley, California 94720, USA

Two-dimensional topological insulators represent a recently descovered phase of matter, characterized by an insulating two-dimensional bulk and metallic one dimensional edge states. These edge states are characterized by spin-momentum locking: particles with opposite spin move in opposite direction. When electron-electron interactions are taken into account, the one-dimensional edge states are conveniently described by the so called helical Luttinger liquid. Within the framework of the helical Luttinger liquid we theoretically show that, due

to the absence of Friedel and Wigner parts in the density operator, density-density correlation functions do not exhibit $2k_F$ and $4k_F$ oscillations, while spin-spin correlations show anisotropic planar wave structure, which is enhanced by electron-electron interactions. Moreover, we demonstrate that the most relevant, in the renormalization group sense, impurity potentials, are not able to modify the average local electron density. Finally we show that only magnetic impurities can pin the planar spin density wave.

TT 59.3 Wed 15:00 Poster D

Criticality at the Haldane-insulator charge-density-wave quantum phase transition — Florian Lange, •Satoshi Ejima, and Holger Feshke — Institute of Physics, University of Greifswald, D-17489 Greifswald, Germany

Exploiting the entanglement concept within a matrix-product-state based infinite density-matrix renormalization group approach, we show that the spin-density-wave and bond-order-wave ground states of the one-dimensional half-filled extended Hubbard model give way to a symmetry-protected topological Haldane state in case an additional alternating ferromagnetic spin interaction is added. In the Haldane insulator, the lowest entanglement level features a characteristic twofold degeneracy. Increasing the ratio between the nearest-neighbor and local Coulomb interaction V/U, the enhancement of the entanglement entropy, the variation of the charge, spin, and neutral gaps, and the dynamical spin and density response signal a quantum phase transition to a charge-ordered state. Below a critical point, which belongs to the universality class of the tricritical Ising model with central charge 7/10, the model is critical with $c = 1/2$ along the transition line. Above this point, the transition between the Haldane insulator and charge-density-wave phases becomes first order.

TT 59.4 Wed 15:00 Poster D

Electron correlations in a one-dimensional manganite model — •Ole Schumann[1], Salvatore R. Manmana[1], Peter E. Blöchl[2], Fabian Biebl[1], and Sangeeta Rajpurohit[2] — [1]Institute for Theoretical Physics, Georg-August-University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institute for Theoretical Physics, TU Clausthal, Leibnizstr. 10, 38678 Clausthal-Zellerfeld

An effective 1D model for a manganite is derived for the ground state atomic structure which consists of antiferromagnetically coupled manganese dimers in the spin triplet state. The model is Hubbard like with an additional staggered magnetic field. Using the DMRG, we obtain the $T = 0$ phase diagram of the resulting many electron model. We investigate various scenarios for photo-excitation of the system and give an outlook to a more realistic modelling.

Financial support via DFG through CRC 1073 "Atomic scale control of energy conversion", project B03 is gratefully acknowledged.

TT 59.5 Wed 15:00 Poster D

Acceleration of MPS-based algorithms by using the adaptive cross approximation — •Holger Thyen, Thomas Köhler, Salvatore R. Manmana, and Stephan Kramer — Institut für Theoretische Physik, Georg-August-Universität, Göttigen

We investigate the benefits of the adaptive cross approximation (ACA) [1], used for the low-rank approximation of the matrices occurring in MPS-based DMRG algorithms. By connecting convergence criteria occurring during the ACA to the discarded weight of the approximation via the usual singular value decomposition (SVD), we obtain a stopping criterion for the iterations of the ACA and investigate possible alternative control parameters. The so obtained code based on ACA is benchmarked to codes based purely on SVD. The code development is part of the open-source SciPAL library [2].

Financial support via DFG through CRC 1073 "Atomic scale control of energy conversion", project B03 is gratefully acknowledged.

[1] M. Bebendorf and S. Rjasanow, Computing **70** 1, (2003).
[2] Stephan C. Kramer and Johannes Hagemann, ACM Trans. Parallel Comput. **1**, 2, Article 15 (2015)

TT 59.6 Wed 15:00 Poster D

Mott quantum criticality in the anisotropic 2D Hubbard model — •Benjamin Lenz[1], Salvatore R. Manmana[1], Thomas Pruschke[1], Fakher F. Assaad[2], and Marcin Raczkowski[2,3] — [1]Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany — [2]Institute for Theoretical Physics and Astrophysics, Julius-Maximilians-Universität Würzburg, Germany — [3]Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Germany

We present evidence for Mott quantum criticality in an anisotropic two-dimensional system of coupled Hubbard chains at half-filling. In this scenario emerging from variational cluster approximation and cluster dynamical mean-field theory, the interchain hopping $t_\perp$ acts as control parameter driving the second-order critical endpoint T_c of the metal-insulator transition down to zero at $t_\perp^c/t \simeq 0.2$. Below $t_\perp^c$ the volume of hole and electron Fermi pockets of a compensated metal vanishes continuously at the Mott transition. Above $t_\perp^c$ the volume reduction of the pockets is cut off by a first-order transition. We discuss the relevance of our findings to a putative quantum critical point in layered organic conductors whose location remains elusive so far.

Financial support via DFG through FOR1807 is gratefully acknowledged.

TT 59.7 Wed 15:00 Poster D

Functional renormalization group studies of spin-orbit entangled j=1/2 Mott insulators — •Finn Lasse Buessen and Simon Trebst — Institute for Theoretical Physics, University of Cologne, Germany

We apply a recently developed functional renormalization group (FRG) approach to study the collective phenomena of spin-orbit entangled j=1/2 moments in Mott insulators. The microscopic exchange of these moments can be captured by a Heisenberg-Kitaev model for various lattice geometries. We discuss technical aspects of the application of the pseudo-fermion FRG approach developed by Reuther and Wölfle and its efficient numerical implementation. Model systems to be discussed include the Heisenberg-Kitaev model on honeycomb and triangular lattice geometries, for which we discuss the formation of unconventional magnetism in the form of spin liquids or non-trivial spin textures.

TT 59.8 Wed 15:00 Poster D

Spin textures in j=1/2 Mott insulators on the triangular lattice — •Tilman Disselkamp and Simon Trebst — University of Cologne

Spin-orbit entangled j=1/2 Mott insulators can give rise to unconventional forms of magnetism, which has sparked an interest in Heisenberg-Kitaev models thought to capture their essential microscopic interactions. Our focus is on j=1/2 Mott insulators in triangular lattice geometries relevant, e.g. to $Ba_3IrTi_2O_9$, for which we study the interplay of geometric frustration and spin-orbit coupling. While the pure Heisenberg model is known to exhibit 120 degree order, non-trivial spin textures are induced by an infinitesimal Kitaev coupling or a Dzyaloshinskii-Moriya exchange. The former stabilizes a $\mathbb{Z}_2$ vortex phase, while the latter gives rise to a skyrmion lattice. Using numerical simulation techniques, we map out the stability of these spin textures at zero and finite temperatures.

TT 59.9 Wed 15:00 Poster D

Scaling theory and universal critical behavior of topological phase transition — •Wei Chen, Markus Legner, and Manfred Sigrist — ETH Zurich, Switzerland

Topologically ordered systems are characterized by topological invariants that are often calculated from the momentum space integration of a certain curvature function, such as Berry curvature or Berry connection. Akin to stretching a messy string to reveal the number of knots it contains, a scaling procedure is proposed for the curvature function, from which one obtains the RG flow of the driving energy parameter (hopping, chemical potential, Coulomb interaction, etc) that distinguishes topological phase transitions. Several critical exponents are further identified from the critical behavior of the curvature function, and the relation between them is explored.

TT 59.10 Wed 15:00 Poster D

Inversion symmetry induced topological edge states in quantum wires — •Sudhakar Pandey[1] and Carmine Ortix[1,2] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — [2]Institute for Theoretical Physics, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands

We demonstrate the existence of topologically non-trivial insulating phases in quantum wires as a consequence of inversion symmetry. The topologically non-trivial phases are characterized by a pair of in-gap edge states which are robust against weak disorder. We find that these topological edge states are identical to the so called Maue-Shockley sur-

face states that can be predicted independently from the location of boundaries and the sign of the Fourier component which opens the insulating gap. We demonstrate that the insulating state can be switched between topologically non-trivial and trivial phases by suitably adjusting the controllable parameters of the Hamiltonian.

TT 59.11 Wed 15:00 Poster D

Breakdown of the bulk boundary correspondence in a strongly correlated model Hamiltonian — •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 bulk boundary correspondence of a archetypal model for interacting Z_2 topological insulators, namely the Kane-Mele-Hubbard model, in particular focusing on the competition between topological and magnetic order. Both bulk and ribbon Green's functions have been calculated using the variational cluster approach, employing a two-site dynamical impurity approximation (DIA). The Z_2 invariant of the bulk can be calculated with a Wannier charge center approach by mapping the interacting system to a topological Hamiltonian, which is an effective free-particle model with the same topological properties. The resulting invariants are compared to the existence of gapless edge states of the ribbon, where we use a site-dependent antiferromagnetic Weiss field on the ribbon. It turns out that spontaneous symmetry breaking occurs locally at the edges already at much smaller interactions than in the middle of the ribbon, leading to a gap in the edge spectral function. As a consequence, the topological invariant defined in the bulk may not correspond to the existence of gapless edge states since time reversal invariance is locally broken only at the edges.

TT 59.12 Wed 15:00 Poster D

Trivial and topological phases protected by symmetries in spin-2 quantum chains — •Augustine Kshetrimayum[1], Hong-Hao Tu[2], and Román Orús[1] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

Symmetry-protected trivial (SPt) phases of matter are the product-state analogue of symmetry-protected topological (SPT) phases. This means, SPt phases can be adiabatically connected to a product state by some path that preserves the protecting symmetry. Moreover, SPt and SPT phases can be adiabatically connected to each other when interaction terms that break the symmetries protecting the SPT order are added in the Hamiltonian. It is also known that spin-1 SPT phases in quantum spin chains can emerge as effective intermediate phases of spin-2 Hamiltonians. In this work, we show that a similar scenario is also valid for SPt phases. More precisely, we show that for a given spin-2 quantum chain, effective intermediate spin-1 SPt phases emerge in some regions of the phase diagram, these also being adiabatically connected to non-trivial intermediate SPT phases. We characterize the phase diagram of our model by studying quantities such as the entanglement entropy, symmetry-related order parameters, and 1-site fidelities. Moreover, we provide a field theory description of the quantum phase transitions between the SPt phases.

TT 59.13 Wed 15:00 Poster D

Raman spectroscopic signature of fractionalized excitations in β-Li_2IrO_3 — •A. Glamazda[1], S.-H. Do[1], K.-Y. Choi[1], and P. Lemmens[2] — [1]Department of Physics, Chung-Ang University, Seoul, Republic of Korea — [2]IPKM, TU-BS, Braunschweig

The Kitaev honeycomb spin model is known to host exotic fractionalized quasiparticles. Using polarization resolved Raman spectroscopy we study the hyper-honeycomb compound β-Li_2IrO_3, a promising candidate of a three-dimensional Heisenberg-Kitaev system. A dynamical Raman response exhibits a broad scattering continuum with distinct polarization, which evolves into a quasielastic response with increasing temperature. The given experimental results give a signature of two-particle Majorana spinon excitations and demonstrate that β-Li_2IrO_3 is close in realizing a three-dimensional Kitaev spin liquid.

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

TT 59.14 Wed 15:00 Poster D

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

Like in the famous oxide heterostructure $LaAlO_3/SrTiO_3$ (LAO/STO) a two dimensional electron system is found at the interface between the strongly correlated Mott insulator $LaTi^{3+}O_3$ and the band insulator STO. In contrast to LAO, the stabilization of $LaTi^{3+}O_3$ requires strong reducing growth conditions since the thermodynamically stable bulk phase is the oxygen-rich $La_2Ti_2^{4+}O_7$. Therefore, we have systematically studied the impact of oxidizing and reducing background atmospheres and the influence of the substrate on $LaTi^{3+}O_3$ thin film growth by pulsed laser deposition. *In situ* x-ray photoelectron spectroscopy of the films prepared on STO exhibit overoxidation probably due to oxygen out-diffusion from the STO substrate, which is reduced for growth on $DyScO_3$ due to the lower oxygen mobility. In addition, we found that a LAO capping layer of a few unit cells thickness acting like a diffusion barrier for oxygen prevents the LTO film from overoxidation during storage in air.

TT 59.15 Wed 15:00 Poster D

Oxygen vacancy induced two-dimensional electron system in disordered-crystalline $LaAlO_3/KTaO_3$ heterostructures — •Michael Zapf[1], Judith Gabel[1], Philipp Scheiderer[1], Lenart Dudy[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

Two-dimensional electron systems (2DESs) in oxide heterostructures based on $SrTiO_3$ are considered to be a promising platform for future microelectronic technology. A variety of interesting properties such as ferromagnetism, resistive switching and superconductivity are linked to interfacial n-doping involving oxygen vacancies. The introduction of a high Z-cation with large spin-orbit coupling like Ta offers an exciting new parameter. We report on a new oxygen vacancy induced 2DES located at the interface of disordered $LaAlO_3$ and crystalline $KTaO_3$, which exhibits remarkably high electron mobilities and charge carrier concentrations. The number of charge carriers can be readily manipulated by the film thickness and irradiation with intense X-rays. Our synchrotron-based hard X-ray photoemission experiments provide a direct probe of the Ta 5d charge carriers at the buried interface to obtain information on the charge carrier density, its depth distribution, and the band structure.

TT 59.16 Wed 15:00 Poster D

Profiling the interfacial electron gas of $LaAlO_3/SrTiO_3$(111) Heterointerfaces — •Judith Gabel[1], Michael Zapf[1], Philipp Scheiderer[1], Philipp Schütz[1], Ozan Kirilmaz[1], Christoph Schlueter[2], Tien-Lin Lee[2], Claudia Cancellieri[3], Victor Rogalev[1,4], Vladimir Strocov[4], 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 — [3]EMPA, Laboratory of Joining Technologies and Corrosion, Duebendorf, Switzerland — [4]Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland

Akin to the the well established $LaAlO_3$(LAO)/$SrTiO_3$(STO) (001) a two-dimensional electron system (2DES) also forms at the interface between LAO and STO in (111) orientation. In contrast to the (001) samples, the (111) oriented structures are predicted to display highly non-trivial topological properties induced by symmetry breaking and the peculiar real space lattice topology. We have investigated the electronic structure of the LAO/STO (111) heterostructure by hard and resonant soft X-ray photoemission. The momentum-resolved electronic structure of the interface Ti 3d states showcases the distinctive symmetry of the (111) orientation. These measurements as well as angular resolved hard X-ray photoemission measurements of the Ti 2p core level furthermore allow conclusions to be drawn about the spatial extent of the interfacial 2DES.

TT 59.17 Wed 15:00 Poster D

Electronic reconstruction at the interface between the Mott insulator $LaVO_3$ and the band insulator $SrTiO_3$ — •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) the formation of a conducting interface is found 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 favourable $LaV^{5+}O_4$ 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 to 5 unit cells. With LVO being a Mott insulator, passivation by the LAO capping opens the opportunity to study a band-filling controlled Mott insulator to metal transition induced by a purely electrostatic mechanism without interfering overoxidation of the LVO film.

TT 59.18 Wed 15:00 Poster D

Stoichiometry control of $SrVO_3$ thin films grown by pulsed laser deposition — •Philipp Scheiderer, Matthias Schmitt, 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 caused by electron correlation yet wait to be fully harnessed. One suitable candidate for future device applications is the correlated metal $SrVO_3$, which can be prepared by pulsed laser deposition (PLD) on commonly used substrates such as $SrTiO_3$. Sample fabrication by PLD offers a wide variety of possibilities to manipulate the structural and electronic properties of the grown films in a controlled way. Here we report on the manipulation of the cation and oxygen stoichiometry of $SrVO_3$ thin films by tuning the laser flux density of the PLD-ablation process and the oxygen background pressure during growth, respectively. *In situ* photoemission, x-ray diffraction, and temperature dependent resistivity measurements enable us to monitor the structural and electronic changes: Cation off-stoichiometry causes a strong increase of the out-of-plane lattice constant as well as a lower residual resistivity ratio, while excess oxygen is found to induce a shift to higher vanadium valences. After exposure to air a similar shift is detected, indicating an overoxidation of the $SrVO_3$ film.

TT 59.19 Wed 15:00 Poster D

Oxygen vacancies at the spinel/perovskite γ-$Al_2O_3/SrTiO_3$ heterointerface probed by resonant photoelectron spectroscopy — •Philipp Schütz[1], Florian Pfaff[1], Michael Zapf[1], Judith Gabel[1], Lenart Dudy[1], Götz Berner[1], Yunzhong Chen[2], Nini Pryds[2], Christoph Schlüter[3], Tien-Lin Lee[3], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Würzburg, Germany — [2]Department of Energy Conversion and Storage, Technical University of Denmark, Risø Campus, Denmark — [3]Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, United Kingdom

The spinel/perovskite heterointerface between the band insulators γ-Al_2O_3 and $SrTiO_3$ hosts a two-dimensional electron system (2DES) with exceptionally high electron mobility. Soft x-ray resonant photoelectron spectroscopy at the Ti L absorption edge is used to probe the Ti $3d$ derived interface states. Marked differences in the resonance behavior are found for the $SrTiO_3$ valence band and the different interface states, which are observed in the band gap of $SrTiO_3$. A comparison to x-ray absorption spectra of Ti $3d^0$ and Ti $3d^1$ systems reveals the presence of different types of electronic states with Ti $3d$ character, i.e., oxygen vacancy induced, trapped in-gap states and itinerant states contributing to the 2DES. Exposure to low doses of oxygen during irradiation allows for the reversible manipulation of the oxygen stoichiometry, thus revealing the presence of an oxygen vacancy-induced state, which is characteristic for this spinel/perovskite interface.

TT 59.20 Wed 15:00 Poster D

2DESs at the surface of locally doped insulating titanates studied by ARPES — •Tobias C. Rödel[1,2], Franck Fortuna[1], François Bertran[2], Thomas Maroutian[3], Philippe Lecoeur[3], 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]Institut d'Electronique Fondamentale, Univ. Paris-Sud, CNRS, Université Paris-Saclay, 91405 Orsay, France

Two-dimensional electron systems (2DESs) in transition metal oxides are currently a field of intense research in the quest of novel functionalities in materials showing competing ground states. The 2DESs in $SrTiO_3$-based interfaces have been the cornerstone of such research. The building block of $SrTiO_3$ and other titanates is the oxygen octahedron. Here we show, using (angle-resolved) photoemission spectroscopy in UHV that the stacking order and the rotation of those octahedra determines the order and hybridization of the t_{2g} orbitals as well as the (de)localized character of the excess electrons in 2DESs. To study different lattice configurations, we characterized the 2DESs at the surface of $SrTiO_3$, $CaTiO_3$ and TiO_2.

TT 59.21 Wed 15:00 Poster D

Thermoelectric and spincaloric properties of epitaxial $LaNiO_3/SrTiO_3$ superlattices from first principles — •Benjamin Geisler[1,2], Ariadna Blanca-Romero[3], and Rossitza Pentcheva[2] — [1]FRM II, Technische Universität München, 85748 Garching, Germany — [2]Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — [3]Imperial College, London, United Kingdom

Modern layer-by-layer fabrication techniques make it possible to grow epitaxial oxide superlattices with atomic precision. By combining accurate DFT+U calculations to determine the atomic and electronic structure and Boltzmann transport theory we show how a targeted design of the interface composition can be used to optimize the thermoelectric and/or spincaloric properties of $LaNiO_3/SrTiO_3(001)$ superlattices. A TiO_2/LaO interface induces n-type doping, and a (potentially highly spin-polarized) charge current arises solely in-plane in the NiO_2 layers. The out-of-plane resistance is high, since the $SrTiO_3$ layers act as tunneling barriers. In contrast, a NiO_2/SrO interface leads to p-type doping. In this case, also the valence band of $SrTiO_3$ contributes to the transmission, thereby reducing the out-of-plane resistance significantly. Besides this doping effect we find that the interface composition influences the electronic band structure, which leads to a nontrivial behavior of the Seebeck coefficient.

Funding by the DFG within TRR 80 (G3 and G8) is acknowledged.

TT 59.22 Wed 15:00 Poster D

Correlated Electronic Properties of Different $SrIrO_3/SrTiO_3$ Heterostructures — •Gernot J. Kraberger and Markus Aichhorn — Institute of Theoretical and Computational Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

Strontium iridates are materials that combine strong electronic correlations with pronounced spin-orbit coupling, giving rise to fascinating physical properties. Strategies to purposefully influence and design these materials are a crucial step to further advance this field. A highly promising candidate for achieving this goal is the formation of heterostructures with other materials. Motivated by this quest, we perform calculations within the DFT+DMFT framework to investigate how the geometry of heterostructures of perovskite $SrIrO_3$ with $SrTiO_3$ influences their correlated electronic structure. We explore the differences between (001)- and (111)-stacked heterostructures, where the latter are particularly interesting because they form buckled honeycomb lattices that have non-trivial topological properties. For the (001)-heterostructures the effect of varying the thickness of the $SrIrO_3$ layers, and thus their effective dimensionality, are studied. As an important ingredient we have to consider the effect of lattice distortions – in the form of a rotation of the oxygen cages – on the electronic correlations. We argue how the interplay of all these factors together allows a targeted modification of the electronic properties of the material.

TT 60: Frontiers of Electronic Structure Theory: Focus on Topology and Transport (Joint session of DS, HL, MA, MM, O and TT organized by O)

Time: Wednesday 18:15–20:30 Location: Poster A

TT 60.1 Wed 18:15 Poster A

Improving anharmonic vibrational calculations from first principles — •Joseph C.A. Prentice, Bartomeu Monserrat, and Richard J. Needs — TCM Group, Cavendish Laboratory, University of Cambridge, UK

The vibrational self-consistent field (VSCF) method, as described in PRB 87 144302, has had several successes in accurately calculating the anharmonic properties of various materials, such as diamond, ice and solid hydrogen. However, a practical issue with the method is the large number of DFT calculations required to map the Born-Oppenheimer energy surface sufficiently accurately. We look at improvements to the method that reduce this computational load, in particular using data on forces from DFT calculations to improve the accuracy of the mapping. Results using this improved method are presented for competing structures of silicate perovskite under lower mantle conditions. Further improvements, involving the inclusion of n-body coupling between phonons, and their possible implementation are also discussed.

TT 60.2 Wed 18:15 Poster A

Towards a practical implementation of second-order Møller-Plesset perturbation theory for solids — •Xiangyue Liu, Arvid Conrad Ihrig, Sergey Levchenko, Igor Ying Zhang, and Matthias Scheffler — *Fritz-Haber-Institut der MPG, Berlin, DE*

The second-order Møller-Plesset perturbation theory (MP2) method is gaining attention in materials science, because it is free from the one-electron self-interaction error. Such error, as a lasting problem in density-functional theory, can lead to a wrong prediction of electronic band gaps, charge transfers, and reaction barriers, all of which are ubiquitous electronic properties or behaviors in condensed-matter systems. However, the unfavourable computational complexity, especially the cubic scaling with respect to the $\boldsymbol{k}$-point number in reciprocal space, limits the applicability of MP2 for solids. In this project we present a practical MP2 implementation for solids in the all-electron full-potential framework. In our implementation, the MP2 correlation energy is evaluated in the atomic-orbital (AO) representation (AO-MP2), which allows for a lower computational scaling in both real and reciprocal spaces[1]. The localized resolution of identity (RI-LVL) technique[2] is adopted to address the memory bottleneck of the AO-MP2 method, making it feasible to handle systems with several hundred atoms per supercell while avoiding the reliance on the disk storage. We demonstrate the accuracy as well as the efficiency of our new MP2 implementation for a diverse set of materials. [1] Levchenko, S. V. *et al.*, Comput. Phys. Comm. **192**, 60, (2015); [2] Ihrig, A.C. *et al.*, New J. Phys. **17** 093020, (2015).

TT 60.3 Wed 18:15 Poster A

Application of the exact exchange functional to magnetic metals within the FLAPW method — •Max Nusspickel[1], Markus Betzinger[1], Christoph Friedrich[1], Andreas Görling[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

Orbital-dependent functionals form a promising class of exchange-correlation (xc) functionals in Kohn-Sham density-functional theory. Already the simplest functional of its kind, the exact exchange functional (EXX), cures the unphysical Coulomb self-interaction error of LDA and GGA functionals. In order to obtain a local xc potential from an orbital-dependent functional, the optimized effective potential (OEP) method is used, resulting in an integral equation for the potential. This equation, however, determines the potential only up to a constant.

In spin-polarized metals, the alignment of the spin-up and spin-down potentials is obtained by the requirement of electron number conservation: variations of the potential can lead to a change of the Fermi energy and, hence, to a variation of the densities of both electron spins. In this way, the OEP equations for the spin-up and spin-down potentials are coupled and the spin-dependent xc potential is obtained from a single OEP equation. We discuss the extension of our EXX-OEP implementation within the linearized augmented plane-wave (FLAPW) method and show results for prototype magnetic metals.

TT 60.4 Wed 18:15 Poster A

Electric switchable giant Rashba-type spin splitting in bulk PbS — •Bin Shao[1], Wenhui Duan[2], and Thomas Frauenheim[1] — [1]BCCMS, University of Bremen, Bremen, Germany — [2]Institute for Advanced Study, Tsinghua University, Beijing, China

Realizing electric controllable spin is one of the major challenges in the field of spintronics. A promising approach is to utilize so-called Rashba effect, which arises from the spin-orbit coupling under broken inversion symmetry, leading to a momentum-dependent spin splitting in k-space. However, the sizes of this splitting are usually rather small, which hinders the application of this effect in spintronics. In this work, based on density functional calculation, we predict a giant Rashba-type spin splitting in bulk PbS with space group $P6_3mc$. The phonon spectrum calculation gives evidence of the thermal stability of this system. The origin of the giant Rashba effect has been demonstrated from the deviation of the S ion from the inversion symmetric position, leading to an ferroelectric polarization along c axis. By switching the direction of the ferroelectric polarization, the spin directions of bulk carriers governed by the Rashba effect are completely rotated, which grants a potential approach to manipulate the spin of electrons by an external electric field. Moreover, under a reasonable hydrostatic pressure, the system could obtain the inversion symmetry due to the movement of the S ion backwards to symmetric positions. As a result, the system turns into a topological phase with the massless Dirac cone state at the (001) surface.

TT 60.5 Wed 18:15 Poster A

GW+fRG: Towards an fRG enhancement of ab initio calculations — Jannis Ehrlich[1,2], Carsten Honerkamp[1], Christoph Friedrich[2], and •Stephan Blügel[2] — [1]Institut für theoretische Festkörperphysik, RWTH Aachen University, D-52056 Aachen, Germany — [2]PGI-1 and IAS-1, FZJ & JARA, D-52425 Jülich, Germany

Spin excitations in solids are of fundamental interest for a wide variety of phenomena. Most materials-specific theoretical studies are based on the adiabatic treatment of the spin-degees of freedom in the context of DFT. Approaches based on the *GW* approximation include screening effects due to charge fluctuations but neglect vertex corrections and other contributions like magnetic fluctuations. The functional renormalization group (fRG) can overcome these limitations as it resums a different class of diagrams, among them charge and magnetic fluctuations and vertex corrections. We discuss how the equations for two-particle vertices in the fRG contain the *GW* approximation, the Bethe-Salpeter equation (BSE) and the parquet approach on certain levels of approximations. Thus, a fRG calculation of materials properties could be a powerful approach to improve the *GW* and BSE methods already applied in first-principles calculations. By using recently suggested channel decomposition schemes [1,2] the method has gained in flexibility and in potential for tackling more complex tasks. Here we propose first steps to develop the fRG approach for the *ab initio* calculation of materials properties.

[1] C. Husemann, M. Salmhofer, Phys. Rev. B **79**, 195125 (2009).
[2] W. Wang *et al.*, Phys. Rev. B **85**, 035414 (2012).

TT 60.6 Wed 18:15 Poster A

The quantum anomalous Hall effect in HgMnTe — •Jan Böttcher, Christoph Kleiner, and Ewelina M. Hankiewicz — Uni Würzburg, Institut für Theoretische Physik und Astrophysik, Germany

Recently, the quantum anomalous Hall (QAH) effect was predicted to exist in Mn doped HgTe. Within the QAH phase only one edge state remains at an edge due to an opposite coupling of spin to the magnetization. The experimental proof is however still outstanding. The paramagnetic nature of the Mn impurities gives rise to the formation of Landau levels which makes it experimentally challenging to distinguish the QAH from a conventional quantum Hall (QH) state. Based on the BHZ model, we present an extended study of the transition from the quantum spin Hall to the QAH state as well as the QAH to the quantum Hall state. For this purpose, we make use of the finite difference method and compare the results with analytical calculations. Hallmarks of the QAH states in the presence of magnetic fields are discussed. The BHZ model has natural limitations in the

high magnetic field regime. We therefore compare our results with band structure calculations based on the 8x8 Kane Hamiltonian. Signatures in the magnetoresistance are discussed which might open the door to distinguish the QAH from the QH state in future transport experiments.

We acknowledge financial support by the DFG within SFB 1170 "ToCoTronics".

TT 60.7 Wed 18:15 Poster A

Nonconventional screening of the Coulomb interaction in low-dimensional semiconductors and insulators — Ersoy Sasioglu, •Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Screening effects play a fundamental role in determining the exciton binding energy, electron dynamics, and the effective electron-electron interaction in low-dimensional semiconductors and insulators. Experimental observation of the large exciton binding energies and nonhydrogenic Rydberg series in low-dimensional semiconductors indicate an unusual non-local screening of the Coulomb interaction. By means of first-principles calculations in conjunction with the random-phase approximation (RPA) within the FLAPW method we study the screening of the Coulomb interaction in low-dimensional semiconductors and insulators. For this purpose a novel tetrahedron method has been implemented. We show that the screening in these systems deviates substantially from the bulk behavior, i.e., the screened interaction W cannot be expressed by a simple static dielectric constant. We compare the numerical RPA results to analytical functions derived from image-charge models for the isolated slab and for a repeated slab model. We find a nonconventional screening in low-dimensions. This nonconventional screening explains the deviations from the usual hydrogenic Rydberg series of energy levels of the excitonic states in one- and two-dimensional semiconductors and opens up possibilities for fundamental studies of correlation effects in low-dimensional materials.

TT 61: Correlated Electrons: (General) Theory 1

Time: Thursday 9:30–13:00 Location: H18

TT 61.1 Thu 9:30 H18

Collective magnetic excitations in correlated systems: self-consistent dual boson approach — Friedrich Krien[1], Evgeny Stepanov[2], Erik van Loon[2], Andrey Katanin[3], Mikhail Katsnelson[2], Alexey Rubtsov[4], and •Alexander Lichtenstein[1] — [1]University of Hamburg — [2]Radboud University Nijmegen — [3]Institute of Metal Physics, Ekaterinburg — [4]Moscow State University

We propose an efficient dual boson scheme for correlated magnetic systems, which extends the local dynamical mean-field theory to non-local interactions and collective excitations. The theory is fully self-consistent both on the one and on the two-particle level, thus describing the formation of collective magnetic modes as well as the renormalization of electrons and magnons spectra on equal footing. The method employs exact solution of effective impurity model consists of both fermion and spin-boson hybridization functions. We show that the theory is naturally described by a dual Luttinger-Ward functional and obeys the relevant conservation laws for magnetic excitations. We compare numerical results for the Hubbard model with non-local magnetic interactions with extended DMFT solution.

TT 61.2 Thu 9:45 H18

Ab-initio study of the finite temperature magnetism in iron and nickel II — •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]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [2]Peter Grünberg Institut, Forschungszentrum Jülich — [3]Institut für Theoretische Physik, Universität Hamburg — [4]Institute of Solid State Physics, TU Wien — [5]Institute of Metal Physics, Ekaterinburg

The calculation of the ferromagnetic transition temperature of itinerant ferromagnets like iron and nickel has been a very hard problem for theory ever since. This is due to the interplay between strong local interactions and the itinerant character of the electrons. Here we show fully ab-initio DFT+DMFT calculations for bcc-iron and fcc-nickel, using the numerically exact Continuous Time Quantum Monte Carlo method in hybridization expansion. We consider the full cubic Coulomb interaction from cRPA. By discussing the effects of commonly used approximations (density-density and Slater-Kanamori) we find, that the magnetic ordering mechanisms in iron and nickel are very different.

TT 61.3 Thu 10:00 H18

Towards an efficient algorithmic combination of functional renormalization group and dynamical mean field theory — •Demetrio Vilardi[1], Nils Wentzell[2,3], Agnese Tagliavini[2,3], Ciro Taranto[1,3], Alessandro Toschi[2], Sabine Andergassen[3], and Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Vienna University of Technology, Vienna, Austria — [3]University of Tübingen, Tübingen, Germany

We present the advancements in the implementation of a recently proposed scheme for a non-perturbative treatment of strongly correlated fermion systems. This approach, called DMF^{2}RG, combines the local strong-coupling treatment of dynamical mean field theory (DMFT) and the non-local one of functional renormalization group (fRG). In our improved algorithmic implementation the full frequency dependence of the local DMFT vertex is retained in the flow. We show results for the one band 2D Hubbard model and compare them against other techniques.

TT 61.4 Thu 10:15 H18

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 Jülich GmbH, Institute for Advanced Simulation, 52425 Jülich, 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 for dynamical mean-field theory to calculate generalized local susceptibilities. The method is applicable to strongly correlated materials with multi-orbital Hamiltonians. We calculate and store the susceptibilities in a compact form by using a Legendre polynomial representation. Furthermore we extend the local susceptibilities to lattice susceptibilities using the Bethe-Salpeter equation. In the talk we show magnetic susceptibility results for a representative system, $VOMoO_4$.

TT 61.5 Thu 10:30 H18

Analytic Continuation of Quantum Monte Carlo Data: Stochastic Sampling Method — •Khaldoon Ghanem and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

We apply Bayesian inference to the analytic continuation of quantum Monte Carlo (QMC) data from the imaginary axis to the real axis. Demanding a proper functional Bayesian formulation of any analytic continuation method leads naturally to the stochastic sampling method (StochS) as the Bayesian method with the simplest prior, while it excludes the maximum entropy method and Tikhonov regularization.

We present a new efficient algorithm for performing StochS that reduces computational times by orders of magnitude in comparison to earlier StochS methods. We apply the new algorithm to a wide variety of typical test cases: spectral functions and susceptibilities from DMFT and lattice QMC calculations. Results show that StochS performs well and is able to resolve sharp features in the spectrum.

TT 61.6 Thu 10:45 H18

Competition of multiplet and spin-orbit splitting in open-shells — •Qian Zhang and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich

To study the trends in the spectra of open-shells across the periodic table, we perform density functional calculations for atoms and ions. We collect the Slater-Condon and spin-orbit parameters from the resulting self-consistent radial wave functions and potentials. To make

these easily accessible, we provide a simple least squares fitting formula in the spirit of Slater's rules. Given these parameters we calculate the many-body spectra in LS-, intermediate-, and jj-coupling. To assess the relative importance of Coulomb and spin-orbit interactions, we estimate the width of the spectra by calculating the eigen-energy variance of the corresponding Hamiltonian using a simple formula that does not require diagonalizing a complicated many-body Hamiltonian.

TT 61.7 Thu 11:00 H18

High-order diagrammatic expansion for the Gutzwiller wave function — Marc Alexander and •Marcus Kollar — Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg

Variational wave functions can provide insights into the physics of correlated electrons, but even the evaluation of static expectation values is notoriously difficult for many-body Hamiltonians. Usually stochastic or perturbative calculations are required, except for a few exact solutions in one or infinite dimensions. For the single-band Hubbard model a diagrammatic formulation for expectation values with the Gutzwiller wave function was developed [1,2], involving the same Feynman diagrams as ϕ^4 field theory. The Feynman diagrams for the latter problem can be generated by computer [3], which we convert and evaluate to high order for the Gutzwiller wave function. Possible applications to equilibrium and nonequilibrium problems are discussed.

[1] W. Metzner, Z. Phys. B. **77**, 253 (1989)
[2] F. Gebhard, PRB **41**, 9452 (1990)
[3] H. Kleinert et al., PRE **62**, 1537 (2000)

15 min. break

TT 61.8 Thu 11:30 H18

Efficient implementation of the parquet equations – role of the reducible vertex function and its kernel approximation — •Gang Li[1], Nils Wentzell[1,2], Petra Pudleiner[1], Patrik Thunström[1], and Karsten Held[1] — [1]nstitute of Solid State Physics, Vienna University of Technology, A-1040 Vienna, Austria — [2]Institut für Theoretische Physik and CQ Center for Collective Quantum Phenomena, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany

We present an efficient implementation of the parquet formalism which respects the asymptotic structure of the vertex functions at both single- and two-particle levels in momentum- and frequency-space. We identify the two-particle reducible vertex as the core function which is essential for the construction of the other vertex functions. This observation stimulates us to consider a two-level parameter-reduction for this function to simplify the solution of the parquet equations. The resulting functions, which depend on fewer arguments, are coined "kernel functions". With the use of the "kernel functions", the open boundary of various vertex functions in the Matsubara-frequency space can be faithfully satisfied. We justify our implementation by accurately reproducing the dynamical mean-field theory results from momentum-independent parquet calculations. The high-frequency asymptotics of the single-particle self-energy and the two-particle vertex are correctly reproduced, which turns out to be essential for the self-consistent determination of the parquet solutions. The current implementation is also feasible for the dynamical vertex approximation.

TT 61.9 Thu 11:45 H18

High-frequency aysmptotics of the local vertex function: algorithmic implementations — •Agnese Tagliavini[1,2], Nils Wentzell[1,2], Gang Li[2], Ciro Taranto[2,3], Georg Rohringer[2], Karsten Held[2], Alessandro Toschi[2], and Sabine Andergassen[1] — [1]Institut für Theoretische Physik, Eberhard Karls Universität, 72076 Tübingen, Germany — [2]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [3]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany

Local vertex functions are a crucial ingredient of several forefront many-body algorithms in condensed matter physics. However, the full treatment of their frequency dependence poses a huge limitation to the numerical performance. A significant advancement requires an efficient treatment of the high-frequency asymptotic behavior of the vertex functions. We here provide a detailed diagrammatic analysis of the high-frequency asymptotic structures and their physical interpretation. Based on these insights, we propose a frequency parametrization, which captures the whole high-frequency asymptotics for arbitrary values of the local Coulomb interaction and electronic density. We present its algorithmic implementation in many-body solvers based on parquet-equations as well as functional renormalization group schemes and assess its validity by comparing our results for the single impurity Anderson model with exact diagonalization calculations.

TT 61.10 Thu 12:00 H18

Reduced density matrix functional theory via a wave function based approach — •Robert Schade[1], Peter Bloechl[1], and Thomas Pruschke[2] — [1]Institute for Theoretical Physics, Clausthal University of Technology, Clausthal, Germany — [2]Institute for Theoretical Physics, University of Goettingen, Goettingen, Germany

We propose a new method for the calculation of the electronic and atomic structure of correlated electron systems based on reduced density matrix functional theory (rDMFT). The density-matrix functional is evaluated on the fly using Levy's constrained search formalism. The present implementation rests on a local approximation of the interaction reminiscent to that of dynamical mean field theory (DMFT). We focus here on additional approximations to the exact density-matrix functional in the local approximation and evaluate their performance.

Financial support by the DFG Research Unit FOR 1346 "Dynamical Mean-Field Approach with Predictive Power for Strongly Correlated Materials" is gratefully acknowledged.

TT 61.11 Thu 12:15 H18

Entanglement-Continuous Unitary Transformations — •Serkan Sahin and Román Orús — Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany

In this talk we present a new algorithm for quantum many-body systems using continuous unitary transformations (CUT) and tensor networks (TNs). With TNs we are able to approximate the solution to the flow equations that lie at the heart of continuous unitary transformations. We call this method Entanglement-Continuous Unitary Transformations (eCUT). It allows us to compute expectation values of local observables as well as tensor network representations of ground states and low-energy excited states. An implementation of the method is shown for 1d systems using matrix product operators. We show preliminary results for the 1d transverse-field Ising model to demonstrate the feasibility of the method.

TT 61.12 Thu 12:30 H18

Towards an improved duality between tensor network states and AdS spacetime — •Charalampos Papadopoulos and Román Orús — Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany

The conjectured AdS/CFT Correspondence, which states that a Conformal Field Theory (CFT) in Minkowski spacetime has a gravity dual in an asymptotically Anti-de Sitter space (AdS), is one of the best understood examples of the holographic principle, and has important applications in condensed matter physics. Tensor Networks (TNs) are a efficient way to calculate low-energy properties for strongly-correlated quantum many-body systems. The Multi-scale Entanglement Renormalization Ansatz (MERA) is a specific TN for a efficient description of critical quantum systems (CFTs). It was recently suggested that the MERA provides naturally a discretization of AdS spacetime on a lattice. It is however known that a conventional MERA can not reproduce the so-called "Bousso Bound", also called holographic entropy bound, which is a bound on the bulk entropy in spacetime. In this context, our aim is to generalize the proposed AdS/MERA correspondence to a more general AdS/TN duality, where the Bousso bound is satisfied. Progress in this direction as well as connections to strongly correlated systems will be discussed.

TT 61.13 Thu 12:45 H18

DMRG Application in Binary Tree Tensor Networks with Non-Abelian Symmetries — •Claudius Hubig and Ulrich Schollwöck — Department für Physik, LMU München, Germany

The density matrix renormalisation group (DMRG) algorithm and the underlying matrix product state (MPS) state representation have become the workhorse of numerical solid state physics in one dimension. Generalisations to two and more dimensions have been realised as general tensor networks. Of these, binary tree tensor networks preserve most of the favourable properties of MPS while already allowing for a strikingly different entanglement structure. This is in particular relevant in the context of dynamical mean-field theory, where DMRG-based solvers have been employed recently, but were hindered by the one-dimensional structure of MPS.

This contribution discusses the implementation and performance behaviour of DMRG and related methods for binary tree tensor networks which identically conserve both abelian and non-abelian symmetries, such as $U(1)_{Charge}$ and $SU(2)_{Spin}$. Numerical exploitation of these symmetries directly leads to large speed-ups and further simplifies parallelisation over many cores.

TT 62: Focus Session: High Temperature Superconductivity in Hydrides

The discovery of superconductivity at 203 K in H_3S was a big surprise although it was predicted theoretically. While unstable at ambient conditions H_3S is a result of the dissociation of H_2S for an applied pressure in excess of 100 GPa in accordance with structure predictions. The transition temperature can be estimated with high accuracy by Density Functional Theory for superconductors. The symposium comprises results from experimental and theoretical studies.

Organizer: Rudi Hackl (WMI Garching)

Time: Thursday 9:30–12:45 Location: H20

Invited Talk TT 62.1 Thu 9:30 H20

Conventional high temperature superconductivity: from A15 to MgB_2 to H_3S — •Igor Mazin — NRL, Washington, DC

I will review, mostly for the benefits of the younger generation, the history of the half-century long quest for the room-temperature superconductivity, concentrating on the conventional electron-phonon mechanism. I will outline several stages, characterized by different paradigmes, which can be tagged in a Potterian way thus:

(1) A-15 and the concept of an upper bound on T_c
(2) V.L. Ginzburg and the concept of a negative dielectric function
(3) MgB_2 and the concept of doped covalent bonds
(4) H_3S and the room temperature superconductivity
(if the room is in Antarctica).

I am dedicating this talk to the memory of my teacher, Vitaly Ginzburg, on occasion of his 100th birthday.

Invited Talk TT 62.2 Thu 10:00 H20

Conventional superconductivity at 203 K at high pressures — Alexander Drozdov[1], •Mikhail Eremets[1], Ivan Troyan[1], Vadim Ksenofontov[2], and Sergii Shylin[2] — [1]1Max-Planck-Institut fuer Chemie, Hahn-Meitner-Weg 1, 55128 Mainz, Germany — [2]Institut fuer Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universitet Mainz, Staudingerweg 9, 55099 Mainz, Germany.

A search for high, room temperature conventional superconductivity is promising as the Bardeen-Cooper-Schrieffer (BCS) theory in the Eliashberg formulation puts no apparent limits on T_c. Materials with light elements are especially favorable as they provide high frequencies in the phonon spectrum. However only a moderately high T_c = 39 K has been found in this search in MgB_2. We systematically studied metallic hydrogen and covalent hydrogen dominant compounds and found the record T_c of 203 K at pressure 140 GPa in sulfur hydride [1]. We proved occurrence of superconductivity by the sharp drop of the resistivity to zero; the decrease of T_c with magnetic field; the pronounce isotope shift of T_c in D_2S which evidences of a major role of phonons in the superconductivity; and the magnetic susceptibility measurements. The X-ray diffraction data confirmed that the superconductive phase has the predicted bcc structure. This phase can be considered as an atomic hydrogen superconductor stabilized by sulfur.

[1] A. P. Drozdov, M. I. Eremets, I. A. Troyan, V. Ksenofontov, S. I. Shylin, Nature **525**, 73 (2015)

Invited Talk TT 62.3 Thu 10:30 H20

Crystal Structure of 200 K-Superconducting Phase in Sulfur Hydride System — •Mari Einaga[1], Masafumi Sakata[1], Takahiro Ishikawa[1], Katsuya Shimizu[1], Mikhail Eremets[2], Alexander Drozdov[2], Ivan Troyan[2], Naohisa Hirao[3], and Yasuo Ohishi[3] — [1]KYOKUGEN, Graduate School of Engineering Science, Osaka university, Machikaneyamacho 1-3, Toyonaka, Osaka, 560-8531, Japan — [2]Max Planck Institut fur Chemie, Hahn-Meitner-Weg 1, 55128 Mainz, Germany — [3]JASRI/SPring-8, 1-1-1, Sayo-cho, Sayo-gun, Hyogo 679-5198. Japan

Superconductivity with the critical temperature T_c above 200 K has been recently discovered by compression of H_2S (or D_2S) under extreme pressure [1]. It was proposed that these materials decompose under high pressure to elemental sulfur and hydride with higher content of hydrogen which is responsible for the high temperature superconductivity. In this study, we have investigated that the crystal structure of the superconducting compressed H_2S and D_2S by synchrotron x-ray diffraction measurements combined with electrical resistance measurements at room and low temperatures. We found that the superconducting phase is in good agreement with theoretically predicted body-centered cubic structure, and coexists with elemental sulfur, which claims that the formation of $3H_2S \rightarrow 2H_3S + S$ is occured under high pressure [2].

[1] A. P. Drozdov *et al.*, arXiv: 1412.0460 (2014), A. P. Drozdov *et al.*, Nature **525**, 73 (2015)
[2] M. Einaga *et al.*, arXiv: 1509.03156 (2015).

15 min. break

Invited Talk TT 62.4 Thu 11:15 H20

Strong-Coupling Electron-Phonon Superconductivity in H_3S — •Warren E. Pickett[1] and Yundi Quan[2] — [1]University of California Davis, Davis CA, USA — [2]Beijing Normal University, Beijing, China

The superconducting phase of hydrogen sulfide at T_c = 200 K observed by Eremets' group at pressures around 200 GPa is simple bcc Im-3m H_3S. Remarkably, this record high temperature superconductor was predicted beforehand by Duan et al., so the theory would seem to be in place. Here we will discuss why this is not true. Several extremes are involved: extreme pressure, meaning reduction of volume;extremely high H phonon energy scale around 1400 K; unusually narrow peak in the density of states at the Fermi level; extremely high temperature for a superconductor. Analysis of the H3S electronic structure and two important van Hove singularities (vHs) reveal the effect of sulfur. The implications for the strong coupling Migdal-Eliashberg theory will be discussed. followed by comments on ways of increasing T_c in H_3S-like materials.

Invited Talk TT 62.5 Thu 11:45 H20

High-pressure phases of S, Se, and P hydrides and their superconducting properties: Predictions from ab-initio theory — •E. K. U. Gross — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The quest for novel high-temperature superconductors in the family of hydrogen-rich compounds has recently been crowned with the experimental discovery of a record critical temperature of 190 K in a hydrogen-sulfur compound at 200 GPa. In the present contribution, we investigate the phase diagram of the H-S system, comparing the stability of H_nS (n = 1,2,3,4) by means of the minima hopping method for structure prediction. Our extensive crystal structure search confirms the H_3S stoichiometry as the most stable configuration at high pressure. Superconducting properties are calculated using the fully ab-initio parameter-free approach of density functional theory for superconductors. We find a T_c of 180 K at 200 GPa, in excellent agreement with experiment. We also show that Se-H has a phase diagram similar to its sulfur counterpart. We predict H_3Se to be superconducting at temperatures higher than 120 K at 100 GPa. We furthermore investigate the phase diagram of PH_n (n = 1,2,3,4,5,6). The results of our crystal-structure search do not support the existence of thermodynamically stable PH_n compounds, which exhibit a tendency for elemental decomposition at high pressure. Although the lowest energy phases of $PH_{n=1,2,3}$ display T_c values comparable to experiment, it

remains uncertain if the measured values of T_c can be fully attributed to a phase-pure compound of PH_n.

Invited Talk TT 62.6 Thu 12:15 H20

New sulfur hydride H_3S and excellent superconductivity at high — •Tian Cui — State Key Laboratory of Superhard Materials, College of physics, Jilin University, Changchun, P. R. China

It is predicted theoretically that molecular hydrogen would dissociate into an atomic phase with metallic properties at high pressures. Metallic hydrogen is believed to be a room-temperature superconductor. However, metallization of hydrogen is still debates in laboratory. As an alternative, hydrogen-rich compounds are extensively explored since their metallization can happen at relatively lower pressures by means of chemical pre-compressions. Here, a new sulfur hydride H_3S that hardly occur at atmospheric pressure was predicted to be formed at high pressure by two main ways. We also found two intriguing metallic structures with R3m and Im-3m symmetries above 111 GPa and 180 GPa, respectively. Remarkably, the estimated T_c of Im-3m phase at 200 GPa achieves a very high value of 191-204 K, reaching an order of 200 K. Further calculation shown that the H atoms play a significant role in superconductivity. The experimental discovery of superconductivity with a high T_c = 203 K in H-S system at high pressure has verified our theoretically predicted results. Furthermore, the predicted R3m and Im-3m structures have been recently confirmed experimentally by synchrotron XRD.

TT 63: Low-Dimensional Systems: 2D - Theory

Time: Thursday 9:30–13:00 Location: H21

TT 63.1 Thu 9:30 H21

Giant valley drifts in uniaxially strained monolayer MoS_2 — •Udo Schwingenschlögl, Qingyun Zhang, Yingchun Cheng, and Li-Yong Gan — PSE Division, KAUST, Thuwal 23955, Saudi Arabia

Using first-principles calculations, we study the electronic structure of monolayer MoS_2 under uniaxial strain. We show that the energy valleys drift far off the corners of the Brillouin zone (K points), about 12 times the amount observed in graphene. Therefore, it is essential to take this effect into consideration for a correct identification of the band gap. The system remains a direct band gap semiconductor up to 4% uniaxial strain, while the size of the band gap decreases from 1.73 to 1.54 eV. We also demonstrate that the splitting of the valence bands due to inversion symmetry breaking and spin-orbit coupling is not sensitive to strain.

[1] Q. Zhang, Y. Cheng, L.-Y. Gan, and U. Schwingenschlögl, PRB **88**, 245447 (2013)

TT 63.2 Thu 9:45 H21

Coexistence of incommensurate magnetism and superconductivity in the two-dimensional Hubbard model — Hiroyuki Yamase[1,2], •Andreas Eberlein[1,3], and Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]National Institute for Materials Science, Tsukuba, Japan — [3]Department of Physics, Harvard University, Cambridge, USA

We analyze the competition of magnetism and superconductivity in the two-dimensional Hubbard model with a moderate interaction strength, including the possibility of incommensurate spiral magnetic order. Using an unbiased renormalization group approach, we compute magnetic and superconducting order parameters in the ground state. In addition to previously established regions of Néel order coexisting with d-wave superconductivity, the calculations reveal further coexistence regions where superconductivity is accompanied by incommensurate magnetic order.

TT 63.3 Thu 10:00 H21

Physical dipoles and second order perturbation theory for dipolar fermions in two dimensions — •Philipp Lange, Jan Krieg, and Peter Kopietz — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt/Main, Germany

By considering electric physical dipoles, we propose a new regularization for the Fourier transform of the interaction of dipolar fermions in two dimensions. Using this regularization, we calculate the self-energy, the renormalized chemical potential, and the renormalized Fermi surface of dipolar fermions in two dimensions in full second order perturbation theory.

TT 63.4 Thu 10:15 H21

Thermodynamics and renormalized quasiparticles in the vicinity of the dilute Bose gas quantum critical point in two dimensions — •Jan Krieg[1], Simon Streib[1], Dominik Strassel[2], Sebastian Eggert[2], and Peter Kopietz[1] — [1]Goethe-Universität Frankfurt, Deutschland — [2]Technische Universität Kaiserslautern, Deutschland

Using the functional renormalization group and quantum Monte Carlo methods we investigate the region close to the quantum critical point of a dilute two-dimensional boson gas in the normal phase. Decoupling the two-particle interaction in the particle-particle channel and using a simple truncation of the flow equations we derive the leading order logarithmic corrections to pressure, density, and entropy as well as to the effective mass and to the wavefunction renormalization. We find that recent experiments using cold atoms are in good agreement with our results.

TT 63.5 Thu 10:30 H21

Nonlocal density interactions on the honeycomb and bilayer square lattice — •Stefan Wessel and Michael Golor — Institute for Theoretical Solid State Physics, RWTH Aachen University

We consider an efficient scheme to perform sign problem-free determinantal quantum Monte Carlo simulations of Hubbard models with nonlocal density-density interactions on half-filled bipartite lattices, based on a bond-decoupling of the extended interaction terms. We apply our scheme to the Hubbard model on the square lattice bilayer with an interlayer repulsion, and present the ground state phase diagram within the accessible parameter region. In particular, for sufficiently strong interlayer tunneling, we observe the emergence of a direct dimer product state of mixed D-Mott and S-Mott character. We also examine the stability range of this state within strong-coupling perturbation theory. Furthermore, we consider the Hubbard model on the honeycomb lattice with next-nearest-neighbor interactions. Such an interaction is found to enhance both charge density and spin-current correlations within the semimetallic region. However, inside the accessible parameter region, they do not stabilize long-ranged charge density wave order nor a quantum spin Hall state, and the only insulating state that we observe exhibits long-range antiferromagnetism.

TT 63.6 Thu 10:45 H21

Spin spectral functions of a quantum spin liquid phase on the kagome lattice from quantum Monte Carlo — •Maximilian Lohöfer and Stefan Wessel — Institute for Theoretical Solid State Physics

We analyze the dynamical spin structure factor of a spin-$\frac{1}{2}$ XY-model on a kagome lattice with additional ring-exchange terms along the bow-tie plaquettes. This model is known to exhibit a quantum phase transition between a transverse ferromagnetic phase and a gapped Z_2 quantum spin liquid regime for strong ring-exchange interactions. We employ a combination of sign problem-free quantum Monte Carlo simulations and analytic continuation to study the evolution of the dynamical structure factor across the quantum phase transition in order to extract signatures for the spin liquid state in this non-trivial spin model.

TT 63.7 Thu 11:00 H21

Boson-fermion duality for corner entanglement entropies in free field theories — •Johannes Helmes[1,2], Lauren Hayward Sierens[2,3], Anushya Chandran[2], and Roger Melko[2,3] — [1]University of Cologne, Germany — [2]Perimeter Institute, Waterloo, Canada — [3]University of Waterloo, Canada

Subleading corrections to the prevalent area-law of (Rényi) entanglement entropies of critical quantum many-body systems are known to show universal behavior. For gapless systems a logarithmic correction

arises from the presence of corners in the subsystem. Its coefficient is concretely related to the central charge of the stress tensor of the low-energy effective conformal field theory (CFT) and hence counts the underlying degrees of freedom. A surprising duality is revealed in these corner terms of an opening angle $\theta \lesssim \pi$ between free boson and Dirac fermion lattice field theories for reciprocal Rényi indices.

We compute the entanglement entropies via an exact lattice diagonalization supplemented by a numerical linked-cluster expansion. Using these data we show that the duality is also relatively robust for a corner with an opening angle of $\theta = \pi/2$. We furthermore apply our numerical treatment to a variety of other angles θ. The results confirm the scaling of the corner term with $(\theta - \pi)^2$ and shed light on the gradual dissolution of the duality in the limit of small angles.

15 min. break

TT 63.8 Thu 11:30 H21

High-performance functional renormalization group calculations for interacting fermions on the square lattice — •Julian Lichtenstein[1,2], David Sánchez de la Peña[1,2], Stefan A. Maier[1,2,3], and Carsten Honerkamp[1,2] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [2]JARA-FIT, Jülich-Aachen Research Alliance – Fundamentals of Future Information Technology — [3]Institute for Theoretical Physics, University of Cologne, Germany

The truncated unity functional renormalization group (TUfRG) approach is a novel functional renormalization group (fRG) variant. It is based on an exchange parametrization of the two-fermion interaction [1], while the structure of the equations is inspired by the singular-mode functional renormalization group put forward by Wang et al. [2]. On the basis of speedup data gained from our implementation we show that the TUfRG facilitates efficient calculations on a large number of multi-core CPUs. In this context, it will be illustrated that a separation of the underlying equations, as it is done in the TUfRG, is numerically advantageous. In order to discuss strong and weak points of this method, we compare data for the t,t' Hubbard model on the square lattice to those from other fRG methods. Furthermore, we analyze the effect of including longer ranged interactions in addition to the purely local Hubbard interaction.

This work was supported by DFG via RTG1995 'Quantum many-body methods in condensed matter systems'.

[1] C. Husemann and M. Salmhofer, PRB **79**, 195125 (2009)
[2] W. S. Wang et al., PRB **85**, 035414 (2012)

TT 63.9 Thu 11:45 H21

A functional Renormalization Group calculation with high wavevector resolution for extended Hubbard models on the honeycomb lattice — •David Sánchez de la Peña[1], Julian Lichtenstein[1], Stefan Maier[1,2], and Carsten Honerkamp[1] — [1]Institute for Theoretical Solid State Physics, RWTH-Aachen University, D-52056 Aachen, Germany and JARA Fundamentals of Future Information Technologies — [2]Institute for Theoretical Physics, Cologne University, D-50937 Cologne, Germany

Extended Hubbard models on the honeycomb lattice exhibit a rich variety of ordering tendencies at low energies, which manifest themselves as instabilities of the normal state respect to the inclusion of electron-electron interactions. In an attempt to describe the low-energy properties of real materials with such a honeycomb structure, like graphene, we analyze the arising ordering tendencies and corresponding critical scales as a function of doping and interaction parameters. For that matter, we employ a truncated unity functional Renormalization Group treatment (TUfRG), which allows for an unbiased investigation of the competing instabilities arising in the effective low-energy theory starting from a given set of bare Coulomb interactions. Being based on channel decomposed flow equations, the wavevector resolution that can be achieved is much higher than that of N-patch fRG schemes, which also allows the inclusion of a weakly screened long-range Coulomb tail in the bare interactions.

This work was supported by the DFG-SPP 1459 'Graphene'.

TT 63.10 Thu 12:00 H21

Frequency-dependent interactions in a two-patch model — •Timo Reckling and Carsten Honerkamp — Institute for Theoretical Solid State Physics, RWTH Aachen University, 52056 Aachen, Germany

We study a two-patch model for interacting fermions with the functional Renormalization Group (fRG). The goal is to gain insight into the frequency dependence of the effective interaction that is generated in the fRG flow. In our model each interaction component g_i depends on three bosonic transfer frequencies or 3 fermionic frequencies that determine the loop contributions on the r.h.s. of the fRG equations. We discuss the applicability of simplified ansatzes like Lorentzians to describe the frequency dependencies. Moreover, we analyze the influence of the frequency dependence on the critical scales of the flows to strong coupling.

This work is supported by the DFG-RTG 1995 "Quantum many-body methods in condensed matter systems".

TT 63.11 Thu 12:15 H21

Efficiency of the Hybrid Quantum Monte Carlo Method for Hubbard type models. — •Stefan Beyl, Fakher F. Assaad, and Florian Goth — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Deutschland

The Hybrid Quantum Monte Carlo method has the potential advantage of reaching very large system sizes for Hubbard type models since it can scale linearly with the euclidean volume. Here we argue that the performance of the method is strongly dimension dependent. In the one-dimensional case, the fact that the fermion matrix has no zeros leads to a stable algorithm which scales more efficiently than generic auxiliary field method. In two dimensions the fermionic matrix has zeros thereby leading to a breakdown of ergodicity. We propose to use a complex Hubbard Stratonovich transformation to avoid this problem.

TT 63.12 Thu 12:30 H21

Spontaneous breaking of particle-hole-symmetry on a Lieb-lattice — •Johannes S. Hofmann[1], Thomas C. Lang[2,1], Martin Bercx[1], and Fakher F. Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Institute for Theoretical Physics, University of Innsbruck, Austria

We study the t-V-model of spinless fermions on a two dimensional Lieb-lattice at half filling, using both exact diagonalization and continuous-time Quantum Monte Carlo (QMC) methods. The non-interacting model supports a Dirac cone as well as a flat band at the Fermi level. While the flatness is protected by the sub-lattice symmetry, a flat band is also highly susceptible to interaction effects. We find that nearest neighbor Coulomb repulsion leads to spontaneous breaking of the sub-lattice symmetry due to the formation of a charge density wave. In principle, this allows to further investigate the model away from half filling without introducing a sign problem to the QMC. We analyze the critical temperature of the phase transition and study its dependence on the interaction strength.

TT 63.13 Thu 12:45 H21

Finite-Temperature Sensitivity of Entanglement Spectra and Their Numerical Reconstruction from Rényi Entropies — •Wilfried Michel, Peter Broecker, and Simon Trebst — University of Cologne, Germany

Entanglement spectra provide deep insight into the entanglement structure of quantum many-body systems, in particular in the presence of (chiral) topological order. Here we discuss numerical approaches to reconstruct the n lowest eigenvalues of the entanglement spectrum from the first n Rényi entropies including characteristic polynoms, maximum entropy techniques, and a power method. We further discuss the stability of the entanglement spectrum in the presence of thermal fluctuations.

We illustrate our findings for the one-dimensional $S = 1/2$ quantum Heisenberg model in a ladder geometry, which exhibits a quantum phase transition from a symmetry protected phase to a trivial phase.

TT 64: Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 1

Time: Thursday 9:30–13:00 Location: H22

TT 64.1 Thu 9:30 H22

Efficient numerical simulations of many-body localized systems — •Frank Pollmann[1], Vedika Khemani[2], and Shivaji Sondhi1[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]Physics Department, Princeton University, Princeton, NJ 08544, USA

Many-body localization (MBL) occurs in isolated quantum systems when Anderson localization persists in the presence of finite interactions. To understand this phenomenon, the development of new, efficient numerical methods to find highly excited eigenstates is essential. We introduce a variant of the density-matrix renormalization group (DMRG) method that obtains individual highly excited eigenstates of MBL systems to machine precision accuracy at moderate-large disorder. This method explicitly takes advantage of the local spatial structure characterizing MBL eigenstates.

TT 64.2 Thu 9:45 H22

Many-Body Localization in the central spin model — •Daniel Hetterich[1], Maksym Serbyn[2], Norman Yao[2], Frank Pollmann[3], and Björn Trauzettel[1] — [1]Institut für theoretische Physik, Universität Würzburg, Würzburg, Germany — [2]Department of Physics, University of California, Berkeley, USA — [3]Max-Plank-Insitut für Physik komplexer Systeme, Dresden, Germany

The periodic Heisenberg chain model obeys signatures of many-body localization (MBL) that persist the insertion of a central spin, which interacts with all other spins of the periodic chain. To support this statement, we present numerical results for the level repulsion of eigenvalues and for the growth of entanglement entropy of subsystems. We discuss why the central spin is not destroying the transition from the thermal phase to the localized phase. Surprisingly, local observables that measure the central spin only can be used to detect MBL within the whole system. Finally, more realistic modifications of our model are addressed by which we depict the experimental relevance of our results for quantum dots.

TT 64.3 Thu 10:00 H22

Many-body localization dynamics from a one-particle perspective — •Talía Lezama Mergold Love, Soumya Bera, and Jens Hjorleifur Bardarson — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany.

Systems exhibiting many-body localization (Anderson insulators in the presence of interactions) present a novel class of nonergodic phases of matter. The study of entanglement, in terms of both exact eigenstates and its time evolution after quenches, has been useful to reveal the salient signatures of these systems. Similarly to the entanglement entropy of exact eigenstates, the one-particle density matrix can be used as a tool to characterize the many-body localization transition with its eigenvalues showing a Fermi-liquid like step discontinuity in the localized phase. However, this analysis distinguishes the Fock-space structure of the eigenstates from the real space. Here, we present numerical evidence for dynamical signatures of the many-body localized phase for a closed fermionic system, using the one-particle density matrix and its time evolution after a global quench. We discuss and compare our results with the well-known logarithmic spreading of entanglement (a dynamical signature of this phase, absent in the Anderson insulator).

TT 64.4 Thu 10:15 H22

Stroboscopic prethermalization in weakly interacting periodically driven systems — Elena Canovi[1], •Marcus Kollar[2], and Martin Eckstein[1] — [1]Max Planck Research Department for Structural Dynamics, University of Hamburg-CFEL — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg

Time-periodic driving provides a promising route to engineer nontrivial states in quantum many-body systems. However, while it has been shown that the dynamics of integrable systems can synchronize with the driving into a non-trivial periodic motion, generic non-integrable systems are expected to heat up until they display a trivial infinite-temperature behavior. Here we show that a quasi-periodic time evolution over many periods can also emerge in systems with weak integrability breaking, with a clear separation of the timescales for synchronization and the eventual approach of the infinite-temperature state [1]. This behavior is the analogue of prethermalization in quenched systems. The synchronized state can be described using a macroscopic number of approximate constants of motion. We corroborate these findings with numerical simulations for the driven Hubbard model.

[1] E. Canovi, M. Kollar, M. Eckstein, arXiv:1507.00991

TT 64.5 Thu 10:30 H22

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, 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 employs a hybridization expansion of the time evolution operator, including 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, which gives us access to slow dynamics such as, e.g., in the presence of magnetic fields or exchange interactions and to nonequilibrium steady states [3,4]. Here, we present first results of this new scheme for the description of strongly correlated materials in the framework of dynamical mean field theory, including benchmark and new results for the Hubbard and periodic Anderson model.

[1] J. Jin *et al.*, J. Chem. Phys. **128**, 234703 (2008)
[2] R. Härtle *et al.*, PRB **88**, 235426 (2013)
[3] R. Härtle *et al.*, PRB **92**, 085430 (2015)
[4] R. Härtle *et al.*, PRB **90**, 245426 (2014)

TT 64.6 Thu 10:45 H22

Irreversibility in Quantum Many-Body Systems — •Markus Schmitt and Stefan Kehrein — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

The question of thermalization in closed quantum many-body systems has received a lot of attention in the past few years. An intimately related question is whether a closed quantum system shows irreversible dynamics. However, irreversibility and what we actually mean by this in a quantum many-body system with unitary dynamics has been explored very little. In our work we investigate the irreversibility of dynamics in quantum many-body systems by studying echo dynamics. In order to quantify the (ir)reversibility we study the time evolution involving an imperfect effective time reversal. Our measure for the recovery of the initial state are the echo peaks occurring in the time evolution of observables. Specifically, we investigate non-interacting and interacting one-dimensional spin chains. We study the characteristics of the echo peak decay and especially focus on whether this depends on the (non-)integrability of the model.

TT 64.7 Thu 11:00 H22

Unruh effect in nonequilibrium quench dynamics — •Manuel Kreye and Stefan Kehrein — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

Recent experimental advances have opened up the field of nonequilibrium quench dynamics. Of particular importance is the question under what conditions quenched systems reach thermalization. For many-body systems with a quadratic Hamiltonian the time evolution is governed by a Bogoliubov transformation. Interestingly, such a transformation is also found in quantum field theory when coordinates are changed from Minkowski to Rindler space, where the latter is used by an accelerated observer. This transformation leads to the Unruh effect, i.e. the fact that the accelerated observer sees particles at a temperature proportional to acceleration.

We discuss the construction of a quadratic many-body Hamiltonian where the time evolution is governed by exactly the same Bogoliubov transformation that generates the Unruh effect. Our analysis shows that one can achieve thermalization only for half the modes by using a specific many-body Hamiltonian that describes parametric pair production. The time evolution turns out to be quite similar to the one from the Unruh effect.

15 min. break

TT 64.8 Thu 11:30 H22

Statistical analysis of the flow equation method for intermediate flow parameters — •Nils O. Abeling and Stefan Kehrein — Institut für Theoretische Physik, Göttingen, Germany

The flow equation approach is an RG-like method employing continuous unitary transformations to map an initial Hamiltonian to an effective Hamiltonian which takes on a simple banded form [1]. In our work we study the properties of the effective Hamiltonian for intermediate flow parameters when only off-diagonal matrix elements with large energy differences (as compared to the many-body level spacing) have been eliminated. In this case, we show that the diagonal elements already contain the necessary information for a time evolution until a certain maximum time. The remaining off-diagonal matrix elements can be interpreted as a banded random matrix.
[1] F. Wegner, Ann. Phys. **506**, 77 (1994)

TT 64.9 Thu 11:45 H22

Slow relaxing electronic dynamics at the Mott transition — •Sharareh Sayyad and Martin Eckstein — Max Planck Institute for the Structure and Dynamics of Matter, University of Hamburg-CFEL, 22761 Hamburg, Germany

While electron thermalization in metals is usually very fast, we propose a slow-down of the electronic relaxation around the metal-insulator crossover regime. Using nonequilibrium slave-rotor dynamical mean field theory, we studied the one-band Hubbard model, weakly coupled to a dissipative bosonic bath. After a slow quench of the hopping amplitude, the relaxation starts from the bad metal and is headed to the good metal forming the quasiparticle. The timescale of the dynamics is dominated by the spinon equilibrium physics. The spinon evolution goes through a U-turn, governed by a nonmonotonous temperature dependence of the bandwidth in equilibrium. In companion to this evolution, the rotor is forming low-energy spectral weight. Although, before the turning point, the rotor is able to build up the spectral density, it takes time to go along with the spinon after the turn.

TT 64.10 Thu 12:00 H22

Lehmann representation of the nonequilibrium self-energy — •Christian Gramsch[1,2] and Michael Potthoff[1,2] — [1]I. Institute for Theoretical Physics, University of Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

It is shown that the nonequilibrium self-energy of an interacting lattice-fermion model has a unique Lehmann representation. Based on the construction of a suitable non-interacting effective medium, we provide an explicit and numerically practicable scheme to construct the Lehmann representation for the self-energy, given the Lehmann representation of the single-particle nonequilibrium Green's function. This is of particular importance for an efficient numerical solution of Dyson's equation in the context of approximations where the self-energy is obtained from a reference system with a small Hilbert space. As compared to conventional techniques to solve Dyson's equation on the Keldysh contour, the effective-medium approach allows to reach a maximum propagation time which can be several orders of magnitude longer. This is demonstrated explicitly by choosing the nonequilibrium cluster-perturbation theory as a simple approach to study the long-time dynamics of an inhomogeneous initial state after a quantum quench in the Hubbard model on a 10x10 square lattice. We demonstrate that the violation of conservation laws is moderate for weak Hubbard interaction and that the cluster approach is able to describe prethermalization physics.

TT 64.11 Thu 12:15 H22

Real-time dynamics after a parameter quench in the two-dimensional Kondo-lattice model with classical spins — •Lena-Marie Gebauer, Mohammad Sayad, and Michael Potthoff — 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 relaxation of a single localized spin, the associated energy and spin dissipation and retardation effects are studied for a one-dimensional Kondo-impurity system [1]. For the lattice variant of the model in two dimensions, 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 quenches of the exchange coupling constant across different phase boundaries.
[1] M. Sayad, M. Potthoff, NJP (in press), arXiv:1507.08227
[2] S. Yunoki et al., PRL **80**, 845 (1998)

TT 64.12 Thu 12:30 H22

How to guarantee complete positivity in approximations to open-system dynamics: Kraus theorem on the Keldysh contour — •Viktor Reimer[1,2] and Maarten Rolf Wegewijs[1,2,3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany

A fundamental problem in the theory of open quantum systems is how to guarantee that the time-evolution within a nontrivial approximation scheme results in a valid physical mixed state.

Spurred by a crucial work of van Wonderen and Suttorp [1], we present a general framework based on the Kraus representation of the exact reduced system dynamics, in which positivity-, hermicity- and trace-preserving approximations can be systematically formulated. We relate the Kraus operators to the standard real-time Keldysh diagrammatic expansion and identify precisely which partial resummations of such diagrams strictly enforce complete positivity of the density operator. This allows the derivation of time-nonlocal quantum master equations with approximate kernels that strictly preserve complete positivity.
[1] A. J. van Wonderen and L. G. Suttorp, EPL **102**, 60001 (2013)

TT 64.13 Thu 12:45 H22

Nonequilibrium dynamics on Chern bands — Sthitadhi Roy, •Adolfo Grushin, Roderich Moessner, and Masudul Haque — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The experimental realization of lattices with Chern bands in ultracold-atom and photonic systems has motivated the study of time-dependent phenomena, such as spatial propagation on such systems. We show that the transverse response to the force due to a harmonic trap on a wavepacket on a Chern lattice, arising due to the interplay of Berry curvature and band dispersion can be captured accurately if the extent of the wavepacket in momentum space is taken into account, unlike point-particle semiclassics. Moreover, if the wavepacket is prepared with a finite initial momentum, the semiclassical analysis reproduces its motion as long as it has a large overlap with the eigenstates of a single band. Relevant for fermionic systems, we study the dynamical evolution of Chern insulator after subjecting them to local quenches. For open-boundary systems, we show for half-filling that the chiral nature of edge states is manifested in the time-dependent chiral response to local density quenches on the edge. In the presence of power-law traps, we show how to mimic the half-filling situation by choosing the appropriate number of fermions depending on the trap size, and explore chiral responses of edges to local quenches in such a configuration. Our results provide different routes to check dynamically the non-trivial nature of Chern bands.

TT 65: Transport: Molecular Electronics and Photonics 1 (Joint session of CPP, DS, HL, MA, O and TT organized by TT)

Time: Thursday 9:30–13:00 Location: H23

TT 65.1 Thu 9:30 H23

Pulling and Stretching a Molecular Wire to Tune its Conductance — •Gaël Reecht[1,4], Hervé Bulou[1], Fabrice Scheurer[1], Virginie Speisser[1], Fabrice Mathevet[2], César González[3], Yannick J. Dappe[3], and Guillaume Schull[1] — [1]IPCMS, Strasbourg, France — [2]Laboratoire de Chimie des Polymères, Paris, France — [3]CEA IRAMIS, Saclay, France — [4]Freie Universität Berlin, Berlin, Germany

Molecular junctions are perceived as the ultimate step toward the miniaturization of electronic components based on organic materials. Here, a low temperature scanning tunnelling microscope is used to lift a polythiophene wire from a Au(111) surface while measuring the current traversing the molecular junction. Conductance traces recorded during the lifting procedures reveal abrupt increases of the current intensity, which we associate to detachments of the wire subunits from the surface, in apparent contradiction with the expected exponential decrease of the conductance with wire length. With, ab initio simulations we reproduce the experimental data and demonstrate that this unexpected behavior is due to release of mechanical stress in the wire. Therefore, with the high control ability of the STM, by stretching the suspended molecular wire, we are able to tune its conductance properties.

TT 65.2 Thu 9:45 H23

STM-induced luminescence of single molecule junction — •Michael Chong[1], Gael Reecht[1], Hervé Bulou[1], Alex Boeglin[1], Fabrice Mathevet[2], Fabrice Scheurer[1], and Guillaume Schull[1] — [1]Institut de Physique et Chimie des Matériaux de Strasbourg - CNRS - France — [2]Laboratoire de Chimie des Polymères - CNRS - Université Pierre et Marie Curie, Paris, France

Electroluminescence of a single molecule can be induced by means of scanning tunneling microscopy. When a molecule is placed between two metallic electrodes it is necessary to decouple it using thin insulating layers in order to measure its intrinsic luminescence. A direct contact with the electrodes (tip and substrate), necessary if we envision to build single molecule electronic devices, results in quenching or broadening of the fluorescence of the molecule. We use on-surface polymerization to embed a cromphore molecule in a molecular chain. The STM tip is then used to lift the chain in order to decouple the cromophore from the surface yet mantaining a circuit like configuration trough the molecular chain. The current generated by applying a bias to the electrodes excites the cromophore that then exhibits narrow line luminescence and vibronic peaks allowing chemical identification the emitting unit.

Moreover we demonstrate that this configuration allows to control the lifetime of the excited state of the emitting molecule by two orders of magnitude by changing the coupling of the single molecle with the substrate adjusting the tip-sample separation. This system might open the way to electro-plasmonic devices at the single molecule level.

TT 65.3 Thu 10:00 H23

Effects of spin-orbit coupling and many-body correlations in STM transport through copper phthalocyanine — Benjamin Siegert, •Andrea Donarini, and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

The interplay of exchange correlations and spin-orbit interaction (SOI) on the many-body spectrum of a copper phtalocyanine (CuPc) molecule and their signatures in transport are investigated. We first derive a minimal model Hamiltonian in a basis of frontier orbitals which is able to reproduce experimentally observed singlet-triplet splittings; in a second step SOI effects are included perturbatively. Major consequences of the SOI are the splitting of former degenerate levels and a sizable magnetic anisotropy, which can be captured by an effective low-energy spin Hamiltonian. We show that STM-based magnetoconductance measurements can yield clear signatures of both these SOI induced effects.

TT 65.4 Thu 10:15 H23

Conductance trend in linear oligoacenes controlled by quantum size-effects — •Richard Korytar[1], Tamar Yelin[2], Nirit Sukenik[2], Ran Vardimon[2], Bharat Kumar[3], Colin Nuckolls[3], Oren Tal[2], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, Germany — [2]Chemical Physics Department, Weizmann Institute of Science, Rehovot, Israel — [3]Department of Chemistry, Columbia University, New York, United States

In conventional electronics, the conductance of a wire decreases with length according to Ohm's law. In molecular electronics, quantum effects lead to a richer phenomenology. Oligoacenes are organic molecules which consist of (linearly) fused benzene rings. Recently, Yelin et al. [submitted] studied conductance of oligoacenes directly coupled to Ag leads and found increase of conductance with molecular length.

I will show that transport through oligoacenes is governed by a quantum size effect which controls the alignment and width of the lowest unoccupied molecular orbital. These ideas will be supported by first-principles transport calculations using density-functional theory.

Linear oligoacenes are one of the simplest realizations of zig-zag terminated graphene nano-ribbons. In the long-wire limit, I will demonstrate that the conductance as a function of the molecular length shows surprising oscillations with period of approx. 11 rings [1].

[1] R. Korytár, D. Xenioti, P. Schmitteckert, M. Alouani, and F. Evers, Nature Communications **5**, 5000 (2014).

TT 65.5 Thu 10:30 H23

Investigation of charge transfer processes in single crystals based on π-conjugated molecules — •Antonia Morherr[1], Alisa Chernenkaya[2], Sebastian Witt[1], Katerina Medjanik[3], Michael Bolte[1], Martin Baumgarten[4], Harald O. Jeschke[1], Roser Valentí[1], and Cornelius Krellner[1] — [1]Goethe-Universität Frankfurt, 60438 Frankfurt a. M., Germany — [2]Johannes Gutenberg-Universität, 55099 Mainz, Germany — [3]Lund University, MAX-lab, 22100 Lund, Sweden — [4]MPI für Polymerforschung, 55021 Mainz, Germany

Designing new charge transfer (CT) materials for tuning the physical properties ranging from metallicity over superconductivity to Mott insulators and the understanding of mechanisms of CT is of great interest [1]. New CT crystals of π-conjugated molecules as donors can be obtained by physical vapor transport (PVT) [2]. (Fluorinated) tetracyanoquinodimethane (TCNQ-F_x, x=0, 2, 4) was used as acceptor material to grow different CT salts. The crystal structure was detected by X-ray diffraction. Further spectroscopic measurements as infrared and NEXAFS measurements were applied on these single crystals to investigate the CT process. The analysis of N1s and F1s K-edge spectra shows changes for different acceptor strengths. Ab initio calculations for all compounds underline these results. This systematic investigation of CT materials helps to understand the CT process in more detail.

[1] N. Toyota, M. Lang, J. Müller, Low-Dimensional Molecular Metals, Springer-Verlag, Berlin, 2007
[2] B. Mahns et al., Cryst. Growth Des. **14**, 1338 (2014)

TT 65.6 Thu 10:45 H23

Single Molecule Junctions with Epitaxial Monolayer Graphene Electrodes — •Konrad Ullmann[1], Pedro B. Coto[2], Susanne Leitherer[2], Michael Thoss[2], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik und Interdisziplinäres Zentrum für Molekulare Materialien, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) — [2]Institut für Theoretische Physik und Interdisziplinäres Zentrum für Molekulare Materialien, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

To study transport through single molecules, a two dimensional, open-access testbed for individual molecules is desirable. Therefore we use epitaxial monolayer graphene to fabricate electrodes for single molecule junctions. With the help of a feedback-controlled electro-burning process nanometer sized gaps can be formed reproducibly. Using these electrodes, we studied transport through molecules with different anchor groups at low temperatures. Strong similarities in results obtained with the MCBJ-technique underline the high quality of our experimental data. For a fullerene-endcapped molecule we are able to assign features from the I-V characteristics to internal molecular degrees of

freedom [1].
[1] K. Ullmann et al., Nano Lett. **15**, 3512 (2015)

TT 65.7 Thu 11:00 H23

Simulation of Electron Transport through Graphene-Molecule Junctions — •Susanne Leitherer[1], Uwe Frank[1], Konrad Ullmann[2], Pedro B. Coto[1], Heiko 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

Charge transport in single-molecule junctions with graphene electrodes is investigated using a combination of density functional theory (DFT) electronic structure calculations and Landauer transport theory. In particular, we study covalently bonded molecule-graphene junctions as well as junctions, where the molecule is weakly bonded to graphene by van der Waals interaction [1]. Considering different examples for molecular bridges between graphene electrodes, we analyze the transmission probability and current-voltage characteristics. In junctions with zigzag terminated graphene electrodes, we find edge states, which can induce additional transport channels [2]. Furthermore, local conductance properties are investigated in the nanojunctions.
[1] K. Ullmann et al., Nano Lett. **15**, 3512 (2015)
[2] I. Pshenichnyuk et al., J. Phys. Chem. Lett. **5**, 809 (2013)

15 min. break

TT 65.8 Thu 11:30 H23

Electron transport through C_{20} molecular junction — •Shigeru Tsukamoto and Stefan Blügel — PGI-1/IAS-1, Forschungszentrum Jülich and JARA, Jülich, Germany

We present electron transport properties of C_{20} molecular junctions, which are evaluated within the framework of the density functional theory. The C_{20} molecular junctions employed in this work are composed of a pair of Al bulk electrodes and a single C_{20} molecule, which is known as the smallest fullerene molecule. The scattering wave functions of the molecular junctions are calculated by solving the Kohn-Sham equation by means of the over-bridging boundary matching method, which is based on the real-space finite-difference formalism. The transmission properties are extracted from the scattering wave functions and the electron transmissions are evaluated by the Landauer-Büttiker formula. The electron transmissions and the scattering wave functions are further analyzed by using the eigenchannel decomposition technique. As the result of the eigenchannel analysis, although the total transmission value is $\sim 3.0G_0$ at around the Fermi level, more than five transmission channels are found to contribute to the electron transport, and none of the eigenchannels are opened to 100%. From the spatial distributions of the eigenchannels, we can see that the HOMO states of C_{20} molecule, which are three-fold degenerated and occupied to one-third, mainly contribute to the transport. In addition, the LUMO state is also found to contribute as one of the eigenchannels at around the Fermi level. In the talk, we will present electron transport calculations with different molecular orientations.

TT 65.9 Thu 11:45 H23

Quantum interference effect transistor via "Kondo Blockade" in single molecule junctions — •Andrew Mitchell[1] and Jens Paaske[2] — [1]Institute for Theoretical Physics, Utrecht University, 3584 CE Utrecht, The Netherlands — [2]Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark

Single molecule junctions are basic building blocks of molecular electronics devices. The full power of these devices will be realized by exploiting inherent quantum mechanical effects. Two of the most striking quantum phenomena, with no classical analogue, are quantum interference (QI) due to competing electron transport pathways, and the Kondo effect (KE) due to entanglement and strong electronic interactions. Both QI and KE are widely observed in experiments. The description of QI accounts for the complexities of molecular structure, but is typically non-interacting. By contrast, the Anderson impurity model is usually used to describe interactions and the Kondo effect, but totally neglects molecular structure. In this talk I discuss the subtle interplay between QI and KE in a unified theory, showing that a novel gate-tunable "Kondo Blockade" regime can be exploited to realize an efficient quantum interference effect transistor.

TT 65.10 Thu 12:00 H23

Quantitative *ab initio* simulations of nanocarbon-metal extended contacts — •Artem Fediai[1,2], Dmitry Ryndyk[1,2], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden — [2]Center for Advancing Electronics Dresden, TU Dresden — [3]Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany

Recently developed approach presented in [1] allows to get quantitative information about the resistance R_c, effective contact length L_c, and contacts resistance scaling $R_c(L_c)$ in different extended side contacts depending on the electrode material. We apply this approach to find a contact resistance of side CNT-metal contacts, transfer length in graphene-metal contacts and electronic properties of the diodes with CNT channel and asymmetric contacts (with the electrodes made of different metals). These kinds of *ab initio* simulations were previously impossible due to numerical intractability of the side contacts longer then several nanometers. Our approach explicitly uses extended contact model concept, enforced by modular approach. This allows us to overcome numerical problems and understand physical processes in extended contacts.
[1] A. Fediai, D.A. Ryndyk, G. Cuniberti, PRB **91**, 165404 (2015)

TT 65.11 Thu 12:15 H23

Molecular switches for dangling bond circuits — •Thomas Lehmann[1,2], Dmitry A. Ryndyk[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Germany

On the road to atomic-scale electronic circuits, dangling bond wires are promising candidates. Dangling bonds are formed by selectively removing hydrogen from a passivated silicon surface [1,2] and multiple dangling bonds in a row feature extended electronic states. Those quasi 1D surface structures can be used as atomic scale interconnects. In such circuits, molecules, which can controllably passivate or depassivate a dangling bond can provide logical inputs for constructing simple logic elements. In this talk, we present recent studies combining density-functional based approaches with Green function methods of a molecular switch for dangling bond wires on silicon.
[1] T. Hitosugi, T. Hashizume, S. Heike, S. Watanabe, Y.Wada, T. Hasegawa, K. Kitazawa, Jpn. J. Appl. Phys. **36**, L361 (1997)
[2] H. Kawai, F. Ample, Q. Wang, Y. K. Yeo, M. Saeys, C. Joachim, J. Phys. Condens. Matter **24**, 095011 (2012)

TT 65.12 Thu 12:30 H23

Switchable negative differential resistance induced by quantum interference effects in porphyrin-based molecular junctions — •Daijiro Nozaki[1], Lokamani Lokamani[2], Alejandro Santana-Bonilla[2], Arezoo Dianat[2], Rafael Gutierrez[2], Gianaurelio Cuniberti[2], and Wolf Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Physik, Universität Paderborn, Paderborn, Germany — [2]Institute for Materials Science, TU Dresden, Dresden, Germany

Charge transport through a carbon-based molecular switch consisting of different tautomers of metal-free porphyrin embedded between graphene nanoribbons is studied by combining electronic structure calculations and nonequilibrium Green's function formalism. Different low-energy and low-bias features are revealed, including negative differential resistance (NDR) and antiresonances, both mediated by subtle quantum interference effects. Moreover, the molecular junctions can display moderate rectifying or nonlinear behavior depending on the position of the hydrogen atoms within the porphyrin core. We rationalize the mechanism leading to NDR and antiresonances by providing a detailed analysis of transmission pathways and frontier molecular orbital distribution.
[1] D. Nozaki, J. Phys. Chem. Lett. **6**, 3950 (2015).

TT 65.13 Thu 12:45 H23

Base alignment dependence on Seebeck coefficient of DNA: A diagrammatic non-equilibrium transport theory approach — •Yoshihiro Asai[1], Yueqi Li[2], Limin Xiang[2], Julio L. Palma[2], and Nongjian Tao[2] — [1]Research Center for Computational Design of Advanced Functional Materials, AIST, Central 2, Umezono 1-1-1, Tsukuba, Ibaraki 305-8568, Japan — [2]Center for Bioelectronics and Biosensors, Biodesign Institute, Arizona State University, Tempe, Arizona 85287-5801, USA

Theoretical calculation of temperature dependence of transport properties at finite bias voltage and/or at finite temperature gradient re-

quires careful description of low energy excitations. Incorporation of phonon transport and its coupling to electron transport by no means should play a crucial role to describe the low energy physics. One of the authors succeeded to describe theoretically the temperature cross over behavior of the electric conductance found in the experiment of a long oligothiophene single molecular wires. The diagrammatic non-equilibrium transport theory is useful to describe the problem qualitatively. While the necessity of the non-perturbative approach to the problem is clear, it would be interesting to know how far we could go within the perturbative framework given that any reliable non-perturbative approach for the problem is not available at present. Here, we apply the theory to discuss the base alignment dependence of the Seebeck coefficient of DNA in the hopping temperature region. We will make comparative discussions on our theoretical results with our experimental ones.

TT 66: Magnetic Heusler Materials, Semimetals und Oxides (Joint session of MA and TT organized by MA)

Time: Thursday 9:30–12:30 Location: H34

TT 66.1 Thu 9:30 H34

Singular manifestation of square-planar geometry and novel S=$\frac{3}{2}$ state of a iridate Na_4IrO_4 — •Sudipta Kanungo[1], Binghai Yan[1,2], Patrick Merz[1], Claudia Felser[1], and Martin Jansen[3] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187, Dresden, Germany — [3]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

Local environments and valence electron counts primarily determine the electronic states and physical properties of transition metal complexes. For example, square-planar surroundings found in transition oxometalates such as curprates, Nickaltes are usually associated with the d^8 or d^9 electron configuration. In this work, we address an experimentally observed exotic square-planar mono-oxoanion $[IrO_4]^{4-}$ in Na_4IrO_4 with Ir(IV) in d^5 (S=$\frac{3}{2}$ state) configuration, using ab-initio calculations. On contrary, in its 3d counterpart, Na_4CoO_4, Co(IV) is in tetrahedral coordination with S=$\frac{5}{2}$ high spin state. Our ab-initio calculations reveal that the on-site Coulomb interaction U is the essential factor for determining the stability of the local coordination as well as spin state. We find that due to weak Coulomb repulsion of Ir-5d electrons, Na_4IrO_4 form in a square-planar coordination whereas for Na_4CoO_4, Co(IV) is in tetrahedral coordination, due to strong electron correlation at 3d Co site. Following the trend from 5d to 3d, we predict that the intermediate 4d material Na_4RhO_4, if synthesized, may favor tetrahedral coordination but with an S=$\frac{1}{2}$ low spin state.

TT 66.2 Thu 9:45 H34

Influence of extended crystal defects on magnetic moments and magnetocrystalline anisotropy in the Heusler phase Fe_2CoGa — •Georg Krugel, Wolfgang Körner, Daniel F. Urban und Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

In the search for new and cheap rare-earth-free hard-magnetic materials, Heusler phases are promising candidates. Depending on their chemical composition, high Curie temperatures and high magnetizations without rare earth elements can be achieved. By using a computational screening approach, Gillesen et al. [1] identified several Heusler phases with high magnetic moments like Fe_2CoGa or Fe_2CoAl.

However, in order to have a good hard-magnetic material with a defined easy axis a substantial intrinsic crystalline anisotropy is needed. Unfortunately, the Heusler phases with high magnetic moment generally crystallize in the regular or inverse cubic structure with zero anisotropy. Nevertheless, extended crystal defects like stacking faults or grain boundaries may lead to preferred crystal orientations and provide a way for optimizing the magnetic anisotropy through microstructure engineering.

We present a density functional theory study on extended defects in Fe_2CoGa which illustrates how much magnetocrystalline anisotropy can be achieved. Furthermore, the impact of the extended defects on the local magnetic moments and the total magnetization is analyzed.

[1] M. Gillessen and R. Dronskowski, J. Comput. Chem. 30, 1290 (2009)

TT 66.3 Thu 10:00 H34

Introducing magnetic functionality into oxide heterostructures by thermodynamic stabilization: $EuO/SrTiO_3$ — •Patrick Lömker[1], Timm Gerber[1], Andrei Gloskovskii[2], Wolfgang Drube[2], and Martina Müller[1,3] — [1]Forschungszentrum Jülich GmbH, PGI-6, Jülich, Germany — [2]DESY Photon Science, DESY, Hamburg, Germany — [3]Universität Duisburg-Essen, Duisburg, Germany

In order to introduce magnetic functionality into all-oxide heterostructures, we integrated ultra thin films of the ferromagnetic insulator EuO epitaxially on conducting 0.5% Nb doped $SrTiO_3$(001) (Nb:STO).

We circumvented the use of thick buffer layers (e.g. SrO) to prevent over-oxidation of EuO films by making use of the thermodynamic properties of Eu metal to ultimately form EuO. In particular, *in situ* XPS shows that Eu-metal only deposition on Nb:STO leads to the formation of ultrathin stoichiometric EuO films through substrate supplied oxygen. Furthermore, the interplay between oxygen pressure, Eu flux and T_S is utilized to extended stoichiometric growth to larger film thicknesses. For $T_S = 20°C$ we report the formation of fully stoichiometric EuO films, whereas growth at elevated temperature (250-500°C) yields epitaxial integration with sub-ML interfacial Eu_2O_3.

Further analysis by LEED, RHEED and XRD reveals the epitaxial relationship EuO(110)/Nb:STO(100). *Ex situ* magnetic analysis shows bulk-like properties for optimized EuO ultra thin films. Finally, HAXPES experiments were performed at PETRA III confirming the thermodynamical stabilization of ferromagnetic EuO on Nb:STO.

TT 66.4 Thu 10:15 H34

Exchange Bias-Like Effect of an Uncompensated Antiferromagnet — •Bastian Henne, Verena Ney, Mariano de Souza, and Andreas Ney — Johannes Kepler Universität Linz - Austria

Commonly, exchange biasing is evidenced by a field-like *horizontal* shift of the $M(H)$-loop dominated by the FM [1]. In contrast, its microscopic origin is attributed to uncompensated spins, *i.e.*, an excess magnetization, of the antiferromagnet (AFM) exchange coupled to the FM [2]. This infers the presence of an additional *vertical* shift . Experimental observations of this shift are limited to few layered FM/AFM systems (for example [3]) and observations in the absence of a FM are lacking. In this contribution we present antiferromagnetic Co:ZnO as model system in which the uncompensated spins indeed exclusively lead to a vertical shift which is measurable by conventional magnetometry. Our findings pave the way for the exploration of the vertical exchange bias effect in the absence of a FM and the possibility to achieve a finite field-resistant magnetization in an uncompensated AFM.

[1] Nogúes, J. and Schuller, I.K., J. Magn. Magn. Mater. **192**, 203 (1999).

[2] Ohldag, H. *et al.*, Phys. Rev. Lett. **91**, 017203 (2003).

[3] Rana, R. *et al.*, Sci. Rep. **4**, 4138 (2014).

TT 66.5 Thu 10:30 H34

Magnetic properties of Fe doped spinel $CoCr_2O_4$ studied from first principles theory — •Biplab Sanyal, Shreemoyee Ganguly, and Raghuveer Chimata — Department of Physics and Astronomy, Uppsala University, Box-516, 75120 Uppsala, Sweden

We present a systematic study of the effects of Fe doping on the electronic and magnetic structures of spinel $CoCr_2O_4$ by ab initio density functional theory and Monte Carlo simulations. Our calculated magnetic structure for pristine $CoCr_2O_4$ correctly reproduces the experimental one with a q-vector of (0.67, 0.67,0.0). We show that the non-collinear spin structure with a non-zero q-vector in the spinel structure is driven towards collinearity by Fe doping by a complex interplay between interatomic exchange interactions. In the inverse spinel structure with 100 % Fe doping, a collinear antiferromagnetic order develops along with a half metallic electronic structure, which evolves due to the chemical disorder between Fe and Co in the B sites described by the coherent potential approximation. To the best of our knowledge,

this is the first comprehensive theoretical study to understand the evolution of magnetic and electronic properties of multiferroic $CoCr_2O_4$ doped with Fe.

15 min. break

TT 66.6 Thu 11:00 H34

Thermodynamic Stability and Control of Oxygen Reactivity at Magnetic Oxide Interfaces: EuO on ITO — •Timm Gerber[1], Patrick Lömker[1], Bernardus Zijlstra[1], Claire Besson[2], David Müller[1], Willi Zander[3], Jürgen Schubert[3], Mihaela Gorgoi[4], and Martina Müller[1,5] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Jülich, Germany — [2]Institut für Anorganische Chemie, RWTH Aachen University, Germany — [3]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, Jülich, Germany — [4]Helmholtz-Zentrum für Materalien und Energie GmbH, Berlin, Germany — [5]Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany

As a prototypical all-oxide heterostructure, the ferromagnetic insulator europium monoxide (EuO) is synthesized on transparent and conductive indium tin oxide (ITO) virtual substrates. Non-destructive hard X-ray photoelectron spectroscopy (HAXPES) is employed to depth profile the chemical composition of the magnetic layer and the buried oxide-oxide interface. We find that the otherwise well-established adsorption-controlled EuO growth mode is not applicable here due to thermally activated oxygen diffusion from ITO. We present how to control the oxygen reactivity at the interface and discuss its origin in a thermodynamic analysis. Our complementary methodical strategy allows for a significant improvement of ultrathin EuO films with sizeable magnetic properties. Generally, our approach derives guidelines for the proper choice of oxide substrates and buffer layer materials for functional all-oxide heterostructures.

TT 66.7 Thu 11:15 H34

Ti_2MnZ (Z=Al, Ga, In) compounds: Nearly spin gapless Semiconductors — •Hongying Jia[1,2], Xuefang Dai[2], and Guodong Liu[2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]School of Material Sciences and Engineering, Hebei University of Technology, Tianjin 300130, P. R. China

Spin gapless semiconductors with-low spin magnetic moments are promising functional materials due to their fascinating potential for realistic applications. The ideal spin gapless semiconductors exhibit zero magnetic moment and low external magnetic fields, leading to smaller energy losses. However, spin gapless semiconductors with zero magnetic moments are rarely reported up to now. Therefore, it is necessary to clarify the differences in the origin of the band gap in two spin channels for spin gapless magnetic semiconductors with Heusler structure. In our work [1], the electronic, structural and magnetic properties of Ti_2MnZ (Z=Al, Ga, In) compounds were systematically investigated using first-principles calculations. Our results demonstrate that these compounds are nearly spin gapless semiconductors and have a zero magnetic moment. The origin of the band gap in different spin directions will be discussed in detail. Besides, the effects of the lattice parameter and doping effects of the congeners on the width of the band gaps are demonstrated. These results will help to better understand the mechanism of spin gapless semiconductors and therefore promote the design of new spin gapless semiconductors.

[1] H. Y. Jia *et al.*, AIP Advances **4**, 047113 (2014)

TT 66.8 Thu 11:30 H34

Contributions from conduction electrons and localized moments to the magnetization in Cu_2MnAl as separated by spin polarized measurements — •Josef Andreas Weber[1], Andreas Bauer[1], Peter Böni[1], Hubert Ceeh[1], Stephen Dugdale[2], Atsuo Kawasuso[4], Michael Leitner[3], Christian Pfleiderer[1], and Christoph Hugenschmidt[1,3] — [1]Physik-Department, Technische Universität München, James-Franck Straße, 85748 Garching, Germany — [2]H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK — [3]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany — [4]Advanced Science Research Center, Japan Atomic Energy Agency, 1233 Watanuki, Takasaki, Gunma 370-1292, Japan

The distinction between localized and itinerant ferromagnetism is for some systems still a contentious issue. In Mn based Heusler systems it is usually assumed, that all the magnetic moments are localized at the Mn atoms. However it was shown, that in Cu_2MnAl there exist different Fermi surfaces for the majority and minority spin channel and therefore also the conduction electrons contribute substantially to the the total magnetic moment [1]. Here we report our results obtained by comparing spin polarized 2D-ACAR measurements with recent magnetic Compton scattering measurements and with spin polarized positron lifetime experiments.

[1] J. A. Weber et al., Phys. Rev. Lett. **115** 206404 (2015).

TT 66.9 Thu 11:45 H34

Chemical disorder as engineering tool for magnetic properties and spin-polarization in Mn3Ga-based Heusler systems — •Lukas Wollmann, Stanislav Chadov, Sunil Wilfred D'Souza, Gerhard H. Fecher, and Claudia Felser — Max-Planck-Insitute for Chemical Physics of Solids

The present contribution discusses the effect of random substitution of Mn in Mn_3Ga as a constructive disorder phenomenon, which, for instance, allows to chemically control the spin-polarization of the charge carriers. It is based on *spin-selective electron localization* encountered by the first-principles calculations on the family of tetragonal Mn-based Heusler materials $Mn_{3-x}Y_xGa$ [1,2]. Our calculations indicate that *spin-selective localization* can be introduced by substituting Mn with almost any 3d transition metal element (Sc, Ti, V, Cr, Fe, Co, Ni, Cu) as well as with several heavier species as Os, Ir or Pt. The spin-polarization was derived from the spin-projected residual conductivity tensor computed within the Kubo-Greenwood formalism within the SPR-KKR method [3], which properly accounts for the effects of electron localization induced by the scattering due to chemical disorder. In this way one might obtain the series of highly spin-polarized alloys with noticeable magnetocrystalline anisotropy, combining the advantages of tetragonal and cubic Heusler compounds.

[1] S. Chadov *et al.*, Phys. Rev. B **91** 094203 (2015); [2] L. Wollmann *et al.*, J. Phys. D: Appl. Phys. **48** 164004 (2015); [3] H. Ebert *et al.*, Rep. Prog. Phys. **74** 096501 (2011).

TT 66.10 Thu 12:00 H34

Yttrium Iron Garnet Thin Films with Very Low Damping Obtained by Recrystallization of Amorphous Material — •Christoph Hauser[1], Tim Richter[1], Nico Homonnay[1], Christian Eisenschmidt[1], Hakan Deniz[2], Dietrich Hesse[2], Stefan Ebbinghaus[1], and Georg Schmidt[1] — [1]Martin-Luther University Halle-Wittenberg, Halle, 06120, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, 06120, Germany

Yttrium Iron Garnet is a room temperature ferrimagnet, which has recently gained importance for magnonics [1]. For the integration into magnonic devices, however very thin films must be used which are mostly fabricated by pulsed laser deposition (PLD) and often suffer from increased damping. Using room temperature deposition and subsequent annealing in an oxygen atmosphere much lower damping can be achieved. For a 56 nm thick layer a damping constant of $\alpha = 6.15 \cdot 10^{-5}$ and a linewidth as small as 1.30 Oe @9.6 GHz are obtained which are the lowest values for PLD grown thin films reported so far. Even for a 20 nm thick layer a damping constant of $\alpha = 7.39 \cdot 10^{-5}$ is found. In this case the FMR linewidth is 3.49 Oe @9.6GHz. The layers show high crystalline quality and sub nanometer surface roughness in various structural characterizations. Our results not only present a method of depositing thin film YIG of unprecedented quality but also open up new options for the fabrication of thin film complex oxides or even other crystalline materials. We are going to present the results of various experiments using different layer thicknesses and annealing parameters. [1]Chumak et al. Nat. Commun. 5, 4700 (2014).

TT 66.11 Thu 12:15 H34

Competing Superexchange Interactions in Sr2-xCaxCoOsO6 Double Perovskite Osmates — •Ryan Morrow[1,2], Rohan Mishra[1], Oscar D. Restrepo[1], Molly R. Ball[1], Wolfgang Windl[1], Sabine Wurmehl[2,3], Ulrike Stockert[2,3], Bernd Büchner[2,3], Jiaqiang Yan[4], Michael A. McGuire[4], John W. Freeland[5], Daniel Haskel[5], and Patrick M. Woodward[1] — [1]OSU, Columbus, OH, United States — [2]IFW, Dresden, Germany — [3]TUD, Dresden, Germany — [4]ORNL, Oak Ridge, TN, United States — [5]ANL, Argonne, IL, United States

Double perovskites containing mixed transition metal cations have exhibited numerous desirable properties such as colossal magnetoresistance, half metallic transport, and high temperature ferrimagnetism. However, a predictive understanding of the superexchange mechanisms

which control the magnetism of these materials when they are insulating and contained ordered 3d and 4d or 5d transition metals has remained elusive. In this work, the novel insulators Sr2CoOsO6, SrCaCoOsO6, and Ca2CoOsO6 are studied through a combination of AC and DC magnetometry, specific heat, X-ray magnetic circular dichroism, and neutron powder diffraction in order to characterize two antiferromagnetic orders in Sr2CoOsO6, two spin glass transitions in SrCaCoOsO6, and ferrimagnetic ordering in Ca2CoOsO6. The details of the crystal structures will be used to draw connections between the tuning of bonding geometry through chemical pressure and the competition between short and long range superexchange interactions on the resulting magnetic ground states.

TT 67: Oxides and Insulator Surfaces: Structure, Epitaxy and Growth (Joint session of O and TT organized by O)

Time: Thursday 10:30–13:30 Location: H4

Invited Talk TT 67.1 Thu 10:30 H4

Imaging orbitals and defects in superconducting FeSe/$SrTiO_3$ — •Jennifer Hoffman[1,2], Dennis Huang[1], Tatiana Webb[1], Shiang Feng[1], Can-Li Song[1,3], Cui-Zu Chang[4], Jagadeesh Moodera[4], and Efthimios Kaxiras[1] — [1]Harvard University, Cambridge, MA, USA — [2]University of British Columbia, Vancouver, Canada — [3]Tsinghua University, Beijing, China — [4]Massachusetts Institute of Technology, Cambridge, MA, USA

Single-layer FeSe grown epitaxially on $SrTiO_3$ has been shown to superconduct with T_c as high as 100 K, more than a factor of 10 higher than bulk FeSe. This dramatic enhancement motivates intense efforts to understand the superconducting mechanism and to design and fabricate devices. Nematic order, breaking the 4-fold rotational symmetry of the crystal, has been proposed as an important factor in the superconducting phase diagram. Meanwhile, atomic defects, which may pin nematic fluctuations or otherwise perturb superconductivity, can provide important clues into the superconducting mechanism as well as practical routes to superconducting devices. Here we use scanning tunneling microscopy (STM) to search for orbital nematicity in single-layer FeSe/$SrTiO_3$, and to investigate atomic-scale defects which locally influence superconductivity. From quasiparticle interference (QPI) images, we disentangle scattering intensities from the orthogonal Fe $3d_{xz}$ and $3d_{yz}$ bands, and quantitatively exclude pinned nematic orbital order with domain size larger than $\delta r \sim 20$ nm. Furthermore, we identify a prevalent "dumbbell"-shaped atomic-scale defect whose placement could be harnessed to define two-dimensional superconducting devices.

TT 67.2 Thu 11:00 H4

Surface structure of Fe_3O_4(110) investigated by Scanning Tunneling Microscopy and Density Functional Theory. — •Brian Walls, Olaf Lübben, and Igor V. Shvets — School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Dublin 2, Ireland

We have performed a combined Scanning Tunneling Microscopy (STM) and Density Functional Theory (DFT) study of the (110) surface of single crystalline magnetite (Fe_3O_4). The (110)-terminated surface consists of two alternating planes, namely the A and B planes. Previous STM studies of the Fe_3O_4(110) surface have shown an A-plane terminated row reconstruction [1,2]. However, in this work STM measurements reveal not just the row reconstruction, but also an atomically flat surface structure which is present when the rows break. Interestingly, this flat structure lies just ∼3Å below the adjacent rows.

DFT calculations were performed in order to gain an understanding of the flat structure. The calculations indicate that the presence of vacancies leads to an energetically favourable model and a good match between simulated STM images (Tersoff-Hamann scheme) and experimental images.

References:
1. R. Jansen *et al.*, *Surf. Sci.* **328**, 237-247 (1995).
2. G. Maris *et al.*, *Surf. Sci.* **600**, 5084-5091 (2006).

TT 67.3 Thu 11:15 H4

Simulating atomic-scale phenomena on surfaces of unconventional superconductors — •Andreas Kreisel[1], Peayush Choubey[2], Tom Berlijn[3], Brian Andersen[1], and Peter Hirschfeld[2] — [1]Niels Bohr Institute, Denmark — [2]Univ. of Florida, USA — [3]CNMS & CSMD, Oak Ridge Nat. Lab., USA

Interest in atomic scale effects in superconductors has increased because of two general developments: First, the discovery of new materials as the cuprate superconductors, heavy fermion and Fe-based superconductors where the coherence length of the cooper pairs is as small to be comparable to the lattice constant, rendering small scale effects important. Second, the experimental ability to image sub-atomic features using scanning-tunneling microscopy which allows to unravel numerous physical properties of the homogeneous system such as the quasi particle excitation spectra or various types of competing order as well as properties of local disorder. On the theoretical side, the available methods are based on lattice models restricting the spatial resolution of such calculations. In the present project we combine lattice calculations using the Bogoliubov-de Gennes equations describing the superconductor with wave function information containing sub-atomic resolution obtained from *ab initio* approaches. This allows us to calculate phenomena on surfaces of superconductors as directly measured in scanning tunneling experiments and therefore opens the possibility to identify underlying properties of these materials and explain observed features of disorder. It will be shown how this method applies to the cuprate material $Bi_2Sr_2CaCu_2O_8$ and a Fe based superconductor.

TT 67.4 Thu 11:30 H4

Decomposition of the model perovskite $SrTiO_3$ under electrochemical stress — •Christian Rodenbücher, Gustav Bihlmayer, Paul Meuffels, Rainer Waser, and Kristof Szot — Peter-Grünberg-Institut, Forschungszentrum Jülich, 52425 Jülich

Transition metal oxides are the key materials for future energy-efficient electronics in particular for logic and memory devices based on the resistive switching effect. Since the switching effect is related to a local reaction of the oxide to an external gradient of the electrical and chemical potential, we investigate the influence of electrochemical stress on the prototype perovskite $SrTiO_3$. We demonstrate that upon application of a DC voltage under UHV conditions, the surface region of alkaline earth titanates transforms into lower binary oxides with nanoporous structure. By means of IRT, XPS, EDX, HR-TEM, and LC-AFM we present that this transformation takes place at relatively low temperatures and is related to a fundamental macroscopic decomposition of the oxide changing the physical properties of the surface region up to depths of several tens of micrometers. Our results demonstrate that in ternary oxides phase transformations can be induced by gradients of the electrochemical potential using a technologically simple method, which not only opens up a new way for tailoring micro layers of functional transition metal oxides with bespoke properties for optical, electronic and chemical applications but also demonstrates the mutability of metal oxides under electrical stress being relevant for the understanding of the electroforming and switching process in novel memristive devices.

TT 67.5 Thu 11:45 H4

Electronic structure of $CeTiO_4$ — •Lukas Sojka[1] and Dominik Legut[2] — [1]FMMI, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic — [2]IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

Cerium titanate structures offer broad range of technological applications because of their optical and catalytic properties. Cerium titanate can form various phases, which depend on the oxidation state of cerium. Using the first-principle calculations, we identified the ground-state structure of a new found phase, $CeTiO_4$. In analogy with $LaTaO_4$, the calculated enthalpy of formation indicates that the most stable structure is the monoclinic one over the orthorhombic structure, and its stability is by factor four higher than in $LaTaO_4$. Based on the calculated electronic structure we determined optical properties, mechanical properties (elastic constants) and thermodynamical properties of both structures of $CeTiO_4$. The results were obtained using single-electron framework of density functional theory calculations employing the VASP code. our results also indicate that cerium is in the

oxidation state of Ce^{4+}.

TT 67.6 Thu 12:00 H4

DFT calculations of the electronic and atomic structure of metal-oxide nanowires formed on Ir(100) — Florian Mittendorfer[1], Pascal Ferstl[2], Matthias Gubo[2], Klaus Heinz[2], M.Alexander Schneider[2], Lutz Hammer[2], and •Josef Redinger[1] — [1]Inst. of Applied Physics, TU Wien, Vienna, Austria — [2]Lehrstuhl für Festkörperphysik, Univ. Erlangen-Nürnberg, Erlangen, Germany

Recently, a self-organized growth of quasi one-dimensional ordered cobalt oxide nanowires on the Ir(100) surface has been witnessed. By deposition of 1/3 ML Co in oxygen rich conditions nanowires of either CoO_2 or CoO_3 stoichiometry are formed, which bind via oxygen to the Ir substrate and leave the Co chains almost completely decoupled from the substrate. We report on DFT calculations for nanowires of CoO_2 and CoO_3 type as well as their Ni, Fe and Mn analogues. We find a very good agreement with experimental data concerning structural details and predict an electronic structure which is not strictly one-dimensional, despite the structural decoupling of the metal atoms from the substrate. First results of collinear calculations indicate a change of magnetism proceeding from nonmagnetic NiO_2, via ferromagnetic CoO_2 and FeO_2 to antiferromagnetic MnO_2.

TT 67.7 Thu 12:15 H4

Two-Dimensional Iron Tungstate Honeycomb Layers on Pt(111) — •Sascha Pomp[1], David Kuhness[1], Giovanni Barcaro[2], Luca Sementa[2], Alessandro Fortunelli[2], Martin Sterrer[1], Falko P. Netzer[1], and Svetlozar Surnev[1] — [1]Institute of Physics, University of Graz, A-8010 Graz, Austria — [2]CNR-ICCOM & IPCF, Consiglio Nazionale delle Ricerche, I-56124 Pisa, Italy

We report the first example of a 2D ternary oxide layer with a honeycomb geometry identified as FeWO3, which has no bulk analogue. The 2D iron tungstate phase described here has been synthesized in UHV via a solid state reaction of (WO3)3 clusters with a FeO monolayer on a Pt(111) surface. It has been characterized by a variety of surface analytic techniques, involving x-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM), low-energy electron diffraction (LEED) and temperature programmed desorption (TPD), combined with density functional theory (DFT) calculations. Consistent with the experimental results, the DFT calculations show that the FeWO3 layer consists of a mixed layer of Fe and W atoms, formally Fe2+ and W4+ species, sitting in fcc and hcp Pt hollow sites, respectively, and arranged in a (2x2) superstructure. This layer is terminated by oxygen atoms in Fe-W bridging positions, forming a buckled honeycomb lattice. In addition the DFT calculations predict that the 2D FeWO3 layer exhibits ferromagnetic order with a Curie temperature of 95 K, as opposed to the antiferromagnetic behavior in the bulk FeWO4 phase.

TT 67.8 Thu 12:30 H4

In-situ electron microscopy studies of praseodymia on Ru(0001) — •Jon-Olaf Krisponeit[1], Jan Höcker[1], Andreas Schäfer[2], Julian Cambeis[1], Alexei Zakharov[2], Yuran Niu[2], Jens Falta[1], and Jan Ingo Flege[1] — [1]University of Bremen, Bremen, Germany — [2]Lund University, Lund, Sweden

Due to the multiple valence states of rare earth elements, their oxides (REOs) play an important role in catalysis applications. A prominent example is ceria, which is well known for its oxygen storage capacity. Grown as microparticles on Ru(0001), ceria shows an excellent crystalline quality and thermal stability, making it well suited for catalytic model studies. We extend these efforts to the less studied praseodymia, which exhibits an intriguingly complex phase diagram with many stable mixed-valence compounds between Pr_2O_3 and the fully-oxidized PrO_2. Furthermore, praseodymia shows the highest oxygen mobility among the REOs, rendering PrO_x/Ru(0001) an attractive inverse catalyst model system.

We have prepared ultra-thin films of PrO_x/Ru(0001) by reactive molecular beam epitaxy. Here, we present in-situ investigations on local morphology and structure by low energy electron microscopy and micro-illumination diffraction (LEEM/μ-LEED), revealing the nucleation of triangular islands and the formation of rotational domains. Furthermore, we studied the local chemical composition by x-ray absorption spectroscopy in imaging mode (XAS-PEEM) and discuss post-oxidation and reduction processes as identified by x-ray photoelectron spectroscopy (XPS).

TT 67.9 Thu 12:45 H4

Electronic structure of ultra-thin ZnO on Metal substrates — •Bjoern Bieniek[1], Patrick Rinke[2], Oliver T. Hofmann[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Aalto University, Helsinki, Finland — [3]TU Graz, Austria

ZnO is a promising candidate for applications in opto-electronics. For a successful application stable n-type and p-type ZnO would be needed. As for many wide band gap semi-conductors, p-type conductivity is difficult to achieve in ZnO. We propose ZnO ultra-thin films on metal substrates as model systems for investigating p-type conductivity in ZnO. In our investigation of the electronic structure of ultra-thin ZnO films (1 to 4 layers) on the (111) surfaces of Ag, Cu, Pd, Pt, Ni, and Rh by means of DFT with the PBE and HSE06 exchange-correlation functionals we find a novel mechanism to achieve p-type conductivity at the surfaces of ZnO thin films on metal substrates. This mechanism is based on the intrinsic polar nature of ZnO $(000\bar{1})$ films. With increasing thickness the polar character of wurtzite ZnO emerges as the films structurally transform from α-BN to wurtzite. electrons are transferred from the Zn-terminated interface to adjacent layers. The resulting field shifts the electronic states upwards until the Fermi energy, provided by the metal, is reached and the film becomes effectively p-type doped at its surface by pinning the electronic states of the top most layer(s) at the Fermi level. The number of layers necessary to achieve effective p-type doping depends on the metallic substrate. We also discuss intrinsic defects in the ZnO films on metal substrates.

TT 67.10 Thu 13:00 H4

Role of dopants on the performance of metal oxide surfaces for the water oxidation:a DFT+U approach — •hamidreza hajiyani and rossitza pentcheva — Fakultät für Physik and Center of Nanointegration (CENIDE), Universität Duisburg-Essen, 47057, Duisburg

Based on density functional theory calculations including an on-site Coulomb repulsion term, we explore the oxygen evolution reaction (OER) at transition metal oxide surfaces. We address strategies how to reduce the overpotential during OER as well as modification of the band edge positions through dopants. A systematic variation of dopands throughout the 3d, 4d and 5d series in α-Fe_2O_3 (0001) surface unravels trends concerning the role of d-band occupation and orbital polarization. Consistent with previous results, the overpotentials correlate with the binding energy of chemisorbed species within a volcano plot. The underlying mechanisms are discussed by monitoring changes of valence and spin state of the surface cations throughout the intermediate steps of OER. We further generalize our results to other oxide structures such as the spinel. Support by the DFG within priority program SPP1613, project PE883/9-2 and a computational grant at the Leibniz Rechenzentrum are gratefully acknowledged.

TT 67.11 Thu 13:15 H4

DFT study of metallic adsorbates on bulk and thin films of Zirconia — •Wernfried Mayr-Schmölzer, Florian Mittendorfer, and Josef Redinger — Inst. of Applied Physics, TU Wien, Vienna, Austria

Zirconia (ZrO_2) is a material with many interesting properties, making it useful for various technological applications, such as a solid electrolyte in solid-oxide fuel-cells or as an oxygen gas sensor. Therefore, a detailed understanding of adsorption and interface properties of Zirconia is very useful. We present results of DFT calculations for the adsorption of metal adatoms and clusters on bulk surfaces and on thin Zirconia films grown by oxidation of a Pt_3Zr substrate. The calculations were performed using the Vienna Ab-Initio Simulation Package (VASP) employing van-der-Waals density functionals. The bonding and adsorption mechanism was studied for various metal adatoms such as noble Au and Ag as well as reactive Ni and Pd. On bulk surfaces we only find a weak physisorption for noble Au and even weaker for Ag ($\approx$ 0.5eV), while reactive Ni and Pd show significantly higher adsorption energies ($>$ 2.0 eV). On a thin supported ZrO_2 film a general increase of the adsorption energies by more than 0.5 eV is predicted, resulting a chemisorbed state for Ag, wheres Au remains more weakly bound. To investigate mobility and cluster formation of these noble adsorbates we report on the surface diffusion barriers for silver and gold where we find values below 0.5 eV. We also report on the interface energy of silver and gold films of varying thickness on the thin oxide film.

TT 68: Transport: Majorana Fermions

Time: Thursday 10:30–13:00 Location: H19

TT 68.1 Thu 10:30 H19

Edge instabilities of topological superconductors — •Johannes S. Hofmann[1,2], Fakher F. Assaad[1], and Andreas P. Schnyder[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Nodal topological superconductors display zero-energy Majorana flat bands at generic edges. The flatness of these edge bands, which is protected by time-reversal and translation symmetry, gives rise to an extensive ground state degeneracy and a diverging density of states. Therefore, even arbitrarily weak interactions lead to an instability of the flat-band edge states towards time-reversal and translation-symmetry broken phases, which lift the ground-state degeneracy. Here, we employ Monte Carlo simulations combined with mean-field considerations to examine the instabilities of the flat-band edge states of d_{xy}-wave superconductors. We find that attractive interactions induce a complex s-wave pairing instability together with a density wave instability. Repulsive interactions, on the other hand, lead to ferromagnetism mixed with spin-triplet pairing at the edge. We discuss the implications of our findings for experiments on cuprate high-temperature superconductors.

TT 68.2 Thu 10:45 H19

Gate-controlled preparation, manipulation, and readout of Majorana bound states in nanowire networks — •Michael Hell — Division of Solid State Physics and NanoLund, Lund University, Box. 118, S-22100, Lund, Sweden — Center for Quantum Devices and Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark

We present a scheme for the preparation, manipulation, and readout of Majorana zero modes in mesoscopic islands in superconducting nanowires [1]. The key ingredient is to reversibly lock the fermion parity of the islands (stemming from the Majorana modes) to their charge state. This is achieved by gate control over Josephson junctions, complementing earlier proposals based on magnetic flux control, and allows experimental tools from quantum-dot experiments to be applied. Based on recent experimental progress, a sequence of milestones interpolating between zero-mode detection and quantum computing might be realized in the near future, including (1) detection of fusion rules for non-Abelian anyons using either proximal charge sensors or pumped current; (2) validation of a prototype Majorana qubit; and (3) demonstration of non-Abelian statistics. Experiments (1) and (2) can be performed already in a single-wire geometry, while experiment (3) requires branched nanowire structures.

[1] D. Aasen, M. Hell, R. V. Mishmash, A. Higginbotham, J. Danon, M. Leijnse, T. S. Jespersen, J. A. Folk, C. M. Marcus, K. Flensberg, and J. Alicea, arXiv:1511.05153]

TT 68.3 Thu 11:00 H19

Topological phases in superconductor-noncollinear magnet interfaces with strong spin-orbit coupling — •Menke H.[1], Toews A.[1,2], and Schnyder A. P.[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Quantum Matter Institute, University of British Columbia, Vancouver BC, Canada V6T 1Z4

Majorana fermions are predicted to emerge at interfaces between conventional s-wave superconductors and non-collinear magnets. In these heterostructures, the spin moments of the non-collinear magnet induce a low-energy band of Shiba bound states in the superconductor. Depending on the type of order of the magnet, the band structure of these bound states can be topologically nontrivial. Thus far, research has focused on systems where the influence of spin–orbit coupling can be neglected. Here, we explore the interplay between non-collinear (or non-coplanar) spin textures and Rashba-type spin-orbit interaction. This situation is realized, for example, in heterostructures between helical magnets and heavy elemental superconductors, such as Pb. Using a unitary transformation in spin space, we show that the effects of Rashba-type spin-orbit coupling are equivalent to the effects of the non-collinear spin texture of the helical magnet. We explore the topological phase diagram as a function of spin-orbit coupling, spin texture, and chemical potential, and find many interesting topological phases, such as p_x-, $(p_x + p_y)$-, and $(p_x + ip_y)$-wave states. Conditions for the formation and the nature of Majorana edge channels are examined. Furthermore, we study the topological edge currents of these phases.

TT 68.4 Thu 11:15 H19

Real space mapping of Yu-Shiba-Rusinov states of an extended magnetic scatterer on a conventional superconductor — •Markus Etzkorn[1], Matthias Eltschka[1], Berthold Jäck[1], Andreas Topp[1], Christian R. Ast[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The interaction of a local magnetic impurity with a superconductor causes the formation of Yu-Shiba-Rusinov (YSR)states in the vicinity of the impurity. These have recently received increasing attention in the context of Majorana Fermions and other exotic states that might be created from the mutual interplay. YSR states have been extensively studied by scanning tunneling microscopy and so far have been discussed mainly in the limit of point scattering impurities. Here we present our investigations of the local properties of single magnetic Copper-Phthalocynaine molecules on the (5x1) reconstructed, superconducting V(100) surface measured at 15 mK temperature. We find very intense YSR states with energies that depend on the precise absorbtion geometry of the molecule. At the same time we find no indication of a local suppression of the superconducting gap around the impurity. We follow the state evolution in real space for about 3 nm corresponding to about three orders of magnitude in spectral intensity. The spectra display rich structure with local variations in the electron-hole asymmetries. The observed intensity changes in the spectra can not be described on the basis of a single point like scattering potential.

TT 68.5 Thu 11:30 H19

Topological phase diagram of superconducting carbon nanotubes — •Lars Milz, Magdalena Marganska-Lyzniak, and Milena Grifoni — Institut I - Theoretische Physik Universität Regensburg, Germany

The topological superconducting phase diagram of superconducting carbon nanotubes is discussed. Under the assumption of a short-ranged pairing potential, there are two spin-singlet states: an s-wave and an exotic $p + ip$-wave that are possible because of the special structure of the honeycomb lattice. The consequences for the possible presence of Majorana edge states in carbon nanotubes are addressed. In particular, regions in the magnetic field-chemical potential plane possibly hosting localized Majorana modes are discussed.

15 min. break

TT 68.6 Thu 12:00 H19

Using Majorana spin-1/2 representation for the spin-boson model — •Pablo Schad[1], Alexander Shnirman[1], and Yuriy Makhlin[2,3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]L.D. Landau Institute for Theoretical Physics, acad. Semyonov av., 1a, 142432, Chernogolovka, Russia — [3]Moscow Institute of Physics and Technology, 141700, Dolgoprudny, Russia

The Majorana representation for spin operators enables efficient application of field-theoretical methods for the analysis of spin dynamics. Moreover, a wide class of spin correlation functions can be reduced to Majorana correlations of the same order, simplifying their calculation. For the spin-boson model, direct application of this method in the lowest order allows for a straightforward computation of the transverse-spin correlations, however, for the longitudinal-spin correlations it apparently fails in the long-time limit. Here we indicate the reason and discuss, how this method can be used as a convenient and accurate tool for generic spin correlations. Specifically, we demonstrate that accurate results are obtained by avoiding the use of the longitudinal Majorana fermion, and that correlations of the remaining transverse Majorana fermions can be easily evaluated using an effective Gaussian action.

TT 68.7 Thu 12:15 H19

Universal transport characteristics of multiple topological superconducting wires with large charging energy — •Oleksiy

Kashuba[1], Carsten Timm[2], and Björn Trauzettel[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Deutschland — [2]Institut für Theoretische Physik, TU Dresden, 01062 Dresden, Deutschland

The system with multiple Majorana states coupled to the normal lead can potentially support the interaction between Majorana fermions and electrons. Such system can be implemented by several floating topological superconducting wires with large charging energy asymmetrically coupled to two normal leads. The analysis of the renormalization flow shows that there is a single fixed point — the strong coupling limit of isotropic antiferromagnetic Kondo model. The topological Kondo-like interaction leads also to the selective renormalization of the tunneling coefficients, strongly enhancing one component and suppressing others. Thus, charging energy crucially changes the transport properties of the system leading to the universal single-channel conductance independently from the values of the initial leads-wires coupling.

TT 68.8 Thu 12:30 H19

Transport signatures of rotating Majorana bound states — •Luzie Weithofer, Sunghun Park, and Patrik Recher — TU Braunschweig, Germany

Recently, a transport scheme for the detection of the exchange phase of Majorana bound states (MBS) has been proposed in a Corbino-geometry topological Josephson junction, where a tunneling current from a single, static metallic tip to two rotating MBS is calculated in the weak tunneling limit [1]. Here, we systematically investigate the transport properties of this scheme for general temperature and tunneling strengths, and in addition discuss the transport signatures of a setup where two metallic tips are involved.

[1] S. Park and P. Recher, arXiv:1505.07124

TT 68.9 Thu 12:45 H19

Majorana tunneling entropy — •Sergey Smirnov — University of Regensburg, D-93040 Regensburg, Germany

In thermodynamics a macroscopic state of a system results from a number of its microscopic states. This number is given by the exponent of the system's entropy. In non-interacting systems with discrete energy spectra, such as large scale quantum dots, the entropy as a function of the temperature has a plateau shape with integer values of the exponent of the entropy on these plateaus. Plateaus with non-integer values are fundamentally forbidden and would be thermodynamically infeasible.

Here we investigate the entropy of a non-interacting quantum dot coupled via tunneling to normal metals with continuum spectra as well as to topological superconductors. We show [1] that the entropy may have non-integer plateaus if the topological superconductors support weakly overlapping Majorana bound states. This brings a fundamental change in the thermodynamics of the quantum dot whose specific heat acquires low temperature Majorana peaks which should be absent according to the conventional thermodynamics. We also provide a fundamental thermodynamic understanding of the transport properties, such as the linear conductance. Thus, demonstrating thermodynamic signatures of Majorana fermions, we, on the other hand, connect them to other fields, such as transport, advancing their further understanding on a deep fundamental basis.

[1] S. Smirnov, PRB **92**, 195312 (2015).

TT 69: Frontiers of Electronic Structure Theory: Focus on Topology and Transport IV (Joint session of DS, HL, MA, MM, O and TT organized by O)

Time: Thursday 10:30–13:15 Location: H24

Topical Talk TT 69.1 Thu 10:30 H24

Transport phenomena in broken-symmetry metals: Geometry, topology, and beyond — •Ivo Souza — Universidad del País Vasco, San Sebastián, Spain

While topological quantization is usually associated with gapped systems – Chern insulators and topological insulators – it can also occur in broken-symmetry metals, where the Fermi surface (FS) consists of disjoint sheets: the Berry-curvature flux through each sheet is quantized, defining an integer Chern index. Using ferromagnetic bcc Fe as an example, I will describe how the FS Chern numbers are related to the chiral degeneracies ("Weyl points") in the bandstructure. When placed in a static magnetic field, a Weyl (semi)metal will display the chiral magnetic effect (CME), where an electric field pulse $\mathbf{E} \parallel \mathbf{B}$ drives a transient current $\mathbf{j} \parallel \mathbf{B}$. Weyl semimetals with broken inversion and mirror symmetries can also display a "gyrotropic magnetic effect" (GME), where an oscillating magnetic field drives a current and, conversely, an electric field induces a magnetization. The GME is the low-frequency limit of natural optical activity. It is governed by the intrinsic magnetic moment (orbital plus spin) of the Bloch electron on the FS, in much the same way that the anomalous Hall effect and CME are governed by the FS Berry curvature. Like the Berry curvature, the intrinsic magnetic moment should be regarded as a basic ingredient in the Fermi-liquid description of transport in broken symmetry metals.

Topical Talk TT 69.2 Thu 11:00 H24

Dirac Fermions in Antiferromagnetic Semimetal — •Peizhe Tang, Quan Zhou, Gang Xu, and Shou-Cheng Zhang — Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045, USA

The analogues of elementary particles in condensed matter systems have been extensively searched for because of both scientific interests and technological applications. Recently massless Dirac fermions are found to emerge as low energy excitations in the materials named Dirac semimetals. The currently known Dirac semimetals are all nonmagnetic with both time-reversal symmetry T and inversion symmetry P. Here we show that Dirac fermions can exist in one type of antiferromagnetic systems, where T and P are broken but their combination PT is respected. We propose orthorhombic antiferromagnet CuMnAs as a candidate, analyze the robustness of the Dirac points with symmetry protections, and demonstrate its distinctive bulk dispersions as well as the corresponding surface states by ab initio calculations. Our results give a new routine towards the realization of Dirac materials, and provide a possible platform to study the interplay of Dirac-related physics and magnetism.

TT 69.3 Thu 11:30 H24

Spin Hall effect in non-collinear antiferromagnets Mn3X (X=Sn, Ge, Ga) — •Yang Zhang[1,3], Yan Sun[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany

Recently, large anomalous Hall effect (AHE) was realized in non-collinear antiferromagnetic (AFM) compounds Mn3X (X=Sn, Ge, Ga). We have found that the nonzero Berry curvature – origin of the AHE observed – will lead to another topological effect, the spin Hall effect (SHE) in the titled compounds. We have systematically investigated the intrinsic SHE and revealed large spin Hall conductivity [~1000 ((*/e)*(S/cm)], which is comparable to that of the well-know SHE material Pt. Our work present a new family of AFM compounds for the room-temperature spintronic applications.

TT 69.4 Thu 11:45 H24

Electronic reconstruction and anomalous Hall conductivity in 3*d*-oxide honeycomb lattices within the corundum structure — •santu baidya and rossitza pentcheva — Fakultät für Physik and Center of Nanointegration (CENIDE), Universität Duisburg-Essen, 47057 Duisburg

The electronic structure of 3*d* transition metal oxide honeycomb layers confined in the corundum structure (α-Al_2O_3) along the [0001] direction is investigated using density functional theory including an on-site Coulomb term (GGA+U). While in some cases (e.g. $(M_2O_3)/(Al_2O_3)_5$, M=Fe, Co, V, Cr, Ni) the confined geometry preserves the magnetic and electronic ground state properties of the corresponding bulk corundum compound M_2O_3, strong deviations from the bulk behavior are observed in the case of Ti_2O_3 and Mn_2O_3 bilayers. Our results indicate a formation of a quasi two-dimensional electron

gas with a vertical confinement of ∼5 Å for Ti_2O_3 and ∼8.5 Å for Mn_2O_3. As a function of lateral strain $(Ti_2O_3)/(Al_2O_3)_5$ undergoes a metal-to-insulator transition associated with a switching of orbital polarization. In the metallic state the Dirac point can be tuned to the Fermi level by variation of the c/a ratio. Including spin-orbit coupling a finite anomalous Hall conductivity is observed in $(M_2O_3)/(Al_2O_3)_5$ (M=Ti, Mn).

TT 69.5 Thu 12:00 H24

Anomalous hall effect in triangular antiferromagnetic ordered structure — •Hao Yang[1], Sun Yan[2], Felser Claudia[2], Parkin Stuart[1], and Binghai Yan[2] — [1]Max Planck Institute of Microstructure Physics, 06120 Halle(Saale), Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

The anomalous Hall effect (AHE), a fundamental transport phenomenon of electrons in solids, has been believed to appear in ferromagnetic materials. Very recently AHE is revealed in noncollinear antiferromagnetic compounds. In this work, we have systematically investigated the AHE in antiferromagnetic materials Mn3X (X=Ir, Ge, Sn, Ga), where noncollinear 120-degree type antiferromagnetic spin order exists in the quasi-layered lattice. Assisted by the symmetry analysis, we demonstrate the strong anisotropy of the intrinsic anomalous Hall conductivity that is determined by the Berry curvature in the band structure. Our work well interprets recent experiment observations and predicts novel antiferromagnetic material candidates for the spintronic application.

TT 69.6 Thu 12:15 H24

Anomalous Hall conductivity and orbital magnetization as local quantities — •Antimo Marrazzo[1] and Raffaele Resta[2] — [1]THEOS, EPF Lausanne, Switzerland — [2]Dipartimento di Fisica, Univ. Trieste, Italy

Anomalous Hall conductivity (AHC) and orbital magnetization (OM) are—from a theorist's viewpoint—closely related: both have an expression as **k**-space integrals of the appropriate geometrical quantity. The **k** space is an artificial construct: all bulk properties are embedded in the ground state density matrix in **r** space, independently of the boundary conditions. Is it possible to address AHC and OM as local properties, directly in **r** space? For insulators, two recent papers have proved that the answer is affirmative: both AHC (quantized in insulators) and OM can be evaluated from a local formula over bounded samples. A rationale can be found in the "nearsightedness" of the density matrix: but since this is *qualitatively* different in insulators and metals (exponential vs. power law) it is not obvious that the same successful approach can be extended to metals. Using model Hamiltonians, we have performed simulations over 2D bounded metallic flakes, where the T-invariance is broken in two alternative ways: either à la Haldane, or by a macroscopic **B** field. In both cases, our simulations show that the relevant quantity can be extracted from a knowledge of the electron distribution in the bulk region of the sample only. This looks counterintuitive because the OM of a magnetized sample owes to currents localized near its surface; but the key reason for the success of the local approach to AHC and OM is that the formulas are *not* based on currents.

TT 69.7 Thu 12:30 H24

Laser induced DC photocurrents in a Topological Insulator thin film — •Thomas Schumann[1], Nina Meyer[1], Gregor Mussler[4], Eva Schmoranzerová[2], Dagmar Butkovicova[2], Helena Reichlová[3], Lukas Braun[5], Christian Franz[6], Michael Czerner[6], Pertr Němec[2], Detlev Grützmacher[4], Tobias Kampfrath[5], Christian Heiliger[6], and Markus Münzenberg[1] — [1]IfP, EMA University Greifswald, Germany — [2]MFF, Charles University, Prague, Czech Republic — [3]FZU, Prague, Czech Republic — [4]PGI-9, Jülich, Germany — [5]FHI Berlin, Germany — [6]University of Gießen, Germany

Topological Insulators (TI) open up a new route to influence the transport of charge and spin in a surface film via spin-momentum locking [1,2]. It has been demonstrated experimentally [2] that illumination by circularly polarized light can result in excitation of a helicity-dependent photocurrent.We report our recent results on laser induced photocurrents in a terniary 3D TI thin film. The resulting photocurrents are classified after [1,2] and we show that there are at least two signals visible, for example in time dynamics, which behave different in the suggested parameters.

We acknowledge the funding of the DFG via the SPP 1666 Topological Insulators and the joint DAAD PPP Czech Republic project FemtomagTopo. [1]S.D.Ganichev,W.Prettl,J.Phys.: Condens. Matter 15 (2003) R935-R983

[2]J.W.McIver,D.Hsieh,H.Steinberg,P.Jarillo-Herrero and N.Gedik, Nature Nanotechnology 7, 96-100 (2012)

TT 69.8 Thu 12:45 H24

Robustness of exchange protocols of Majorana fermions in quantum wire networks — •Christian Tutschku[1], Rolf W. Reinthaler[1], Chao Lei[2], Allan H. MacDonald[2], and Ewelina M. Hankiewicz[1] — [1]Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany — [2]Department of Physics, University of Texas at Austin, USA

The interface between topological non-trivial, one-dimensional, spinless p-wave superconductors and the vacuum is connected to the appearance of Majorana edge-modes [1], whose non-trivial exchange statistics makes them promising candidates for topological quantum computation [2]. Via T-Bar structures build of 1D-nanowires we can manipulate and exchange the Majorana fermions by purely electrical means [3]. By applying a tight binding approach we solve the time dependent Bogoliubov-de Gennes equations for the Kitaev chain model [1] and also cure the problem of an appearing additional Majorana-boundstate located at the T-Bar crossing point for small lattice constants. Furthermore we analyze how the robustness of the exchange protocols is affected by non-adiabatic effects or by a finite overlap of the Majorana bound states.

We acknowledge financial support by the DFG within SFB 1170 ToCoTronics.

[1] A. Y. Kitaev, Physics-Uspekhi **44**, 131 (2001)
[2] D. A. Ivanov, PRL **86**, 268 (2001)
[3] J. Alicea et al., Nature Physics **7**, 412 (2011)

TT 69.9 Thu 13:00 H24

Unpaired Majorana modes in Josephson junctions arrays with gapless bulk excitations — •Manuel Pino Garcia — Department of Physics and Astronomy, Rutgers The State University of New Jersey, 136 Frelinghuysen rd, Piscataway, 08854 New Jersey, USA

The search for Majorana bound states in solid-state physics has been limited to materials which display a gap in their bulk spectrum. We will show that such unpaired states appear in certain quasi-one-dimensional Josephson junctions arrays with gapless bulk excitations. The bulk modes mediate a coupling between Majorana bound states via the Ruderman-Kittel-Yosida-Kasuya mechanism. As a consequence, the lowest energy doublet acquires a finite energy difference. For realistic set of parameters this energy splitting remains much smaller than the energy of the bulk eigenstates even for short chains of length L ~ 10. In this talk, we first explain the JJA system and how to model it with an Ising-like Hamiltonian. Then, a qualitative argument is employed to obtain the low-energy effective theory using unpaired Majorana modes. We will show numerical results which confirm the validity of this effective theory and discuss problems that may arise in the experimental realization of our proposal.

TT 70: Graphene: Electronic Properties (Joint session of DS, DY, HL, MA, O and TT organized by O)

Time: Thursday 10:30–12:45 Location: S053

TT 70.1 Thu 10:30 S053

PEEM of epitaxial graphene on silicon carbide — •Richard Hönig, Christoph Keutner, Cornelis Hilscher, Ulf Berges, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

Graphene is a promising candidate for two-dimensional electronic structures. Especially epitaxial graphene on silicon carbide (SiC) is in the focus of current studies, due to the well-established infrastruc-

ture for SiC in the semiconductor-industry.

We present photoemission electron microscopy (PEEM) studies of epitaxial graphene, grown by confinement controlled sublimation (CCS). This technique is a suitable tool for producing large areas of homogeneous graphene. The resulting flake-sizes of graphene exceed the resolution of scanning tunneling microscopy. However, the PEEM-technique provides a better suited resolution up to the mesoscopic scale. Hence, PEEM was chosen to study and characterize these graphene/SiC-samples.

Here, we will demonstrate the first characterization procedures and results. In the future, samples with an adequate amount of graphene will be used for further studies, including the real-time imaging of intercalation-processes.

TT 70.2 Thu 10:45 S053

Graphene growth on structured SiC — •Alexander Stöhr[1], Jens Baringhaus[2], Aleixei Zakharov[3], Christoph Tegenkamp[2], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Deutschland — [2]Leibniz-Universität Hannover, Hannover, Deutschland — [3]MAX IV Laboratory, Lund University, Lund, Schweden

Despite its missing band gap, graphene is reviewd as a potential successor of silicon for applications in logical devices. Nowadays, few techniques are available to introduce a band gap into the band structure of graphene. One of the most promising methods is the confinement of its charge carriers into quasi one-dimensional stripes, so called graphene nanoribbons. Unfortunately, the usual approach to structure graphene by lithography techniques leads to disorder and defects at the edges of the nanoribbons, which then dominat the electronic states of the ribbon. To circumvent this problem, we structure our SiC-crystal prior to the graphene growth. After the growth process a faceting of the sidewalls by 23-28° was observed by AFM. On those areas which are inclined towards the non-structured surface, diffraction spots and a π-band were observed in microscopic LEED and ARPES, respectively. Those experimental findings confirm the growth of ordered graphene on the facets.

TT 70.3 Thu 11:00 S053

A new candidate for silicon carbide (3x3) surface reconstruction — •Jan Kloppenburg[1,3], Lydia Nemec[2,3], Björn Lange[4], Matthias Scheffler[3], and Volker Blum[4] — [1]Université catholique de Louvain — [2]Technische Universität München — [3]FHI Berlin — [4]Duke University

Silicon carbide (SiC) is a primary substrate for high quality epitaxial graphene growth. Graphene growth on SiC(000-1) surface is significantly different from the well controlled monolayer graphene growth on the silicon face. On the carbon face, a (3x3) surface as a precursor phase precedes graphene growth changing the thermodynamics compared to the Si-face[1]. Despite more than a decade of research the precise atomic structure of the (3x3) surface reconstruction of SiC(000-1) is still not clear. Here, we employ an *ab initio* random structure search (AIRSS) based on van-der-Waals corrected PBE density functional theory (DFT) to identify the reconstruction in the C-rich range. Our search reveals a new lowest energy surface reconstruction model for the C-rich SiC(000-1) face that was not previously reported[2] and that would explain the very different graphitization behaviour compared to the Si-face. Simulated STM images are in excellent agreement with previously reported experimental findings[3,4].

[1] Nemec et al, *Phys. Rev. Lett.* **111**, 065502, 2013
[2] Nemec et al, *Phys. Rev. B* **91**, 161408, 2015
[3] Hiebel et al, *Phys. Rev. B* **80**, 235429, 2009
[4] Hiebel et al, *Phys. Rev. B* **45**, 154003, 2011

TT 70.4 Thu 11:15 S053

Characterisation of Graphene Electrodes — •Markus Manz[1], Martin Lottner[1], Martin Stutzmann[1], and Jose Garrido[1,2] — [1]Walter Schottky Institut, Technische Universität München, Garching, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain

The biocompatibility and flexibility of graphene devices allow for long-term in vivo detection of action potentials [1]. Thus, graphene has a serious advantage over former approaches [2] using other materials, which are rigid or brittle. Furthermore, the transparency of graphene micro electrodes allows for simultaneous optical stimulation/imaging and electrical recording [1]. While graphene has a high in plane conductivity, the out of plane conductivity of undoped single layer graphene (SLG) is rather low. This is a major drawback for the detection of neurotransmitters through their respective redox reactions. Therefore, various methods have been developed to increase the out of plane conductivity and 'activate' [3] the SLG electrodes. We investigated two methods of graphene 'activation', namely ozonization and doping with nitric acid. We characterized the modified electrodes using cyclic voltammetry, impedance spectroscopy, and Raman spectroscopy. We then compared the sensitivity of the untreated and 'activated' electrodes towards the neurotransmitters norepinephrine and dopamine.

[1] Kuzum, D. et al., Nat. Commun. 5:5259doi: 10.1038/ncomms6259 (2014). [2] Kwon, K. Y. et al. in Biomedical Circuits and Systems Conference (BioCAS), 2012 IEEE 164-167 (2012). [3] Kasry, A. et al., ACS Nano 4, 3839-3844 (2010).

TT 70.5 Thu 11:30 S053

Ultraclean Freestanding Graphene by Pt-metal catalysis — •Jean-Nicolas Longchamp, Conrad Escher, and Hans-Werner Fink — Physics Department of the University of Zurich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

When using graphene as a substrate in electron microscopy, the presence of residues is obstructive because the latter are often of the same size as the object under study. While the growth of defect-free single-layer graphene by means of chemical vapor deposition (CVD) is nowadays a routine procedure, easily accessible and reliable techniques to transfer graphene to different substrates in a clean manner are still lacking. We have discovered a method for preparing ultraclean freestanding graphene using the catalytic properties of platinum metals. Complete catalytic removal of a sacrificial PMMA layer only requires annealing in air at a temperature between 175°C and 350°C. Here, we will describe in detail the preparation process for obtaining ultraclean freestanding graphene by Pt-metal catalysis. The presentation of low-energy electron holography and TEM investigations will demonstrate that areas of ultraclean freestanding graphene as large as 2 microns square can now routinely be prepared.

TT 70.6 Thu 11:45 S053

Nano-scaled graphene solution-gated field-effect transistors — •Peter Knecht[1], Benno Martin Blaschke[1], Karolina Stoiber[1], Martin Letter[1], Simon Drieschner[1], and Jose Antonio Garrido[2] — [1]Walter Schottky Institut, TU München, Garching, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain

Graphene solution-gated field-effect transistors (SGFETs) are a promising biosensing platform, due to their unique properties such as high charge carrier mobility, low electronic noise, good electrochemical performance and an excellent biocompatibility. The recording of cell action potentials using graphene SGFETs has already been demonstrated. However, the sensing area of several hundred square micrometer is not small enough to resolve potential changes on a subcellular level. In this work, we present the fabrication of nano-scaled graphene SGFETs where the transistor area is reduced to 0.01 square micrometer. The dependence of the transistor's transconductance and the electronic low frequency noise on size and shape of the sensing area is studied. In addition, we investigate if the reduced device size leads to a more pronounced dependence of the device's performance on the graphene quality. Finally, the recording of cell action potentials using the nano-scaled devices is demonstrated and compared to micro-scaled graphene SGFETs.

TT 70.7 Thu 12:00 S053

Graphene wrinkles: their conductivity, crystallinity, and reactivity — •Raul D. Rodriguez[1,2], Tao Zhang[3], Jana Kalbacova[1,2], Devang Parmar[1], Akhil Nair[1], Zoheb Khan[1], Mahfujur Rahaman[1], Ihsan Amin[2], Jacek Gasiorowski[1], Evgeniya Sheremet[1], Rainer Jordan[2], Michael Hietschold[1], and Dietrich R.T. Zahn[1,2] — [1]Institut für Physik, Technische Universität Chemnitz, Chemnitz 09107, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Germany — [3]Professur für Makromolekulare Chemie, Department Chemie, Technische Universität Dresden, Mommsenstrasse 4, 01062 Dresden, Germany

Wrinkles appear to be unavoidable in graphene produced by chemical vapor deposition (CVD) on copper. Despite its generality, isolating the role of wrinkles on overall electrical conductivity, crystallinity, and chemical reactivity of CVD-grown graphene remains an open issue. We investigate the reactivity of basal planes and wrinkles in graphene with polystyrene bromide (PSBr) and correlate it with electrical conductivity, defect concentration, and doping with a special resolution from the micro- to the nano-scale. We show that wrinkles dominate

the chemical reactivity of CVD graphene, and moreover, that doping with the same functionality can yield opposite electronic type to the basal plane regions (n- vs. p-type). These results expand our understanding of wrinkles in CVD graphene towards engineering for novel applications.

TT 70.8 Thu 12:15 S053

Conversion of pyrrolyl-thiophenol self-assembled monolayers (SAMs) into carbon nanomembranes (CNMs) and graphene — •Christof Neumann[1], Matthias Füser[2], Michael Mohn[3], Ute Kaiser[3], Andreas Terfort[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Institute of Inorganic and Analytical Chemistry, Goethe University Frankfurt, 60348 Frankfurt — [3]Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm

The conversion of aromatic self-assembled monolayers (SAMs) into carbon nanomembranes (CNMs) and graphene presents a promising pathway to the production of a broad variety of functional 2D materials [1]. The properties of these materials can be flexibly tuned via an appropriate choice of the molecular building units for SAMs. Here we investigate the conversion of 4-(1H-pyrrol-1-yl)thiophenol and 4-(2,5-dimethyl-1H-pyrrol-1-yl)thiophenol SAMs on polycrystalline copper foils into CNMs via the electron induced crosslinking. Furthermore, we study the pyrolytic transformation of these CNMs into graphene at temperatures up to 800 °C. We characterize these different conversion steps and the resulting physical and chemical properties of CNMs and graphene by a number of complementary experimental techniques including X-ray photoelectron and Raman spectroscopy, high-resolution transmission electron and helium ion microscopy as well as by electric transport measurements. [1] P. Angelova et al.,: A Universal Scheme to Convert Aromatic Molecular Monolayers into Functional Carbon Nanomembranes, ACS Nano 7, 6489 (2013)

TT 70.9 Thu 12:30 S053

Extracellular stimulation of electrogenic cells using graphene devices — •Karolina Stoiber[1], Martin Lottner[1], Markus Manz[1], Simon Drieschner[1], Benno Blaschke[1], Martin Stutzmann[1], and José A. Garrido[1,2] — [1]Walter Schottky Institut, Technische Universität München, Garching, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain

Graphene is a highly conductive, chemically stable, flexible and biocompatible material. Therefore, Graphene microelectrode arrays (GMEAs) are a promising bio-sensing and cell stimulation platform in neural implants. In this work, the electrical stimulation of HEK293 and HL1 cells through extracellular voltage trains by GMEAs is presented. Further, the investigation of the biocompatibility of graphene foam and its capability for extracellular stimulation is discussed.

GMEAs with circular electrodes were fabricated using standard photo-lithography techniques. For the characterization of the devices Raman-spectroscopy and cyclic voltammetry were used. The cell membrane potential of HEK293 cells was monitored during extracellular stimulation via patch-clamping. HL1 cells, a cardiomyocyte-like cell line, were dyed with a calcium-sensitive fluorophore and the modulation of their firing frequency upon stimulation was recorded.

Graphene foam devices were fabricated as previously described. The devices were characterized electrochemically and their capability for extracellular stimulation of HL1 cells tested.

TT 71: 2D Materials beyond Graphene -Dynamics and Excitation (Joint session of DS, DY, HL, MA, O and TT organized by O)

Time: Thursday 10:30–13:30 Location: S054

Invited Talk TT 71.1 Thu 10:30 S054

Spin- and Pseudospin-Polarized Excited States in bulk WSe_2 — Roman Bertoni[1], Christopher Nicholson[1], Lutz Waldecker[1], Michele Puppin[1], Claude Monney[2], Cephise Cacho[3], Hannes Huebener[4], Umberto De Giovannini[4], Angel Rubio[4], Martin Wolf[1], and •Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]University of Zurich, Zurich, CH — [3]Rutherford Appleton Laboratory, Didcot, UK — [4]University of the Basque Country, San Sebastian, ES

The peculiar electronic structure of layered semiconducting transition metal dichalgogenides (TMDC) like WSe_2 gives rise to internal quantum degrees of freedom of the electrons in addition to the spin, namely valley and layer pseudospins. Employing XUV-based time- and angle-resolved photoemission spectroscopy (trARPES) with resonant excitation of excitonic transitions, we observe circular dichroism in the excited state population in the K valleys of the topmost trilayer of bulk WSe_2. Such spin-, valley and layer-polarized excitations are a manifestation of broken site symmetry in an inversion-symmetric crystal. The valley- and layer-resolved view on excited state dynamics provided by trARPES is complemented by the investigation of electron-lattice coupling in multilayer WSe_2 with femtosecond electron diffraction. Latter studies reveal the dynamics of global energy transfer from electronic to vibrational degrees of freedom in TMDCs subsequent to excitonic as well as interband excitation.

TT 71.2 Thu 11:00 S054

Exciton dynamics in two-dimensional materials with strong spin-orbit interaction: $MoSe_2$ versus WSe_2 — •Daniel Schmidt[1], Tillmann Godde[2], Johannes Schmutzler[1], Marc Assmann[1], Jörg Debus[1], Freddie Withers[3], Osvaldo Del Pozo-Zamudio[2], Konstantin S. Novoselov[3], Andre Geim[3], Manfred Bayer[1], and Alexander Tartakovskii[2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Department of Physics and Astronomy, University of Sheffield, Sheffield S3 7RH, UK — [3]School of Physics and Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, UK

Monolayers of semiconducting transition metal dichalcogenides such as MoS_2, WS_2, $MoSe_2$ and WSe_2 have attracted considerable attention following the discovery of the indirect-to-direct bandgap transition from bulk to monolayer material and the coupling of spin and valley degrees of freedom in atomically thin layers. An important characteristic of these compounds is the strong spin-orbit interaction, which leads to a splitting between dark and bright exciton sub-bands. A detailed understanding of dark and bright exciton dynamics and non-radiative processes is important for light emitting applications as has been demonstrated in other systems such as phosphorescent organic light emitting diodes. We measure time-integrated and -resolved PL in monolayers of $MoSe_2$ and WSe_2 in a wide range of temperatures from 10 to 300K and gain insights into the exciton and trion dynamics. Our study reveals similar carrier dynamics for both materials, whereas pronounced differences have been observed for the overall PL intensities.

TT 71.3 Thu 11:15 S054

Electron dynamics in eiptaxial single layer MoS_2 — •Antonija Grubisic-Cabo[1], Jill A. Miwa[1], Signe S. Gronborg[1], Jonathon M. Riley[2], Jens C. Johannsen[3], Cephise Cacho[4], Oliver Alexander[4], Richard T. Chapman[4], Emma Springate[4], Marco Grioni[3], Jeppe V. Lauritsen[1], Phil D. C. King[2], Philip Hofmann[1], and Soren Ulstrup[1] — [1]Aarhus University, DK — [2]University of St. Andrews, UK — [3]Ecole Polytechnique Federale de Lausanne, CH — [4]CLF, STFC Rutherford Appleton Laboratory, UK

The current understanding of the optical properties and excited carrier dynamics in single-layer and few-layer transition metal dichalcogenides relies largely on a series of photoluminescence and differential absorption measurements. Since excitons dominate the optical response, the dynamics of free carriers cannot be studied directly. Here, we use time- and angle-resolved photoemission spectroscopy to directly measure free carriers in epitaxial single layer MoS_2 grown on either Au(111) or on graphene. For MoS_2/Au(111) we determine an ultrafast (50 fs) extraction of excited free carriers via the metal and ascertain a direct quasiparticle band gap of 1.95 eV. The observed quasiparticle gap is significantly smaller than the theoretically estimated value for free-standing MoS_2. This can be explained by a strong renormalisation of the band gap. For MoS_2 on graphene, we find indications of induced band shifts that lead to a time-dependence of the electronic structure.

TT 71.4 Thu 11:30 S054

Understanding optical properties of atomically thin semiconductors from a many-body perspective — •Matthias Drüppel, Thorsten Deilmann, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Transition metal dichalcogenides (TMDCs) open the door to a fascinating, fast growing field of two dimensional atomically thin semiconductors. This increases the demand for novel theoretical techniques, which allow to reliably calculate the optical properties in large systems, the inclusion of substrates or even correlation between more than two particles.

We take the state of the art approach of DFT $\rightarrow$ GW $\rightarrow$ Bethe-Salpeter equation (BSE) and apply the efficient LDA+GdW [1] method. This enables us to describe many-body electronic excitations at moderate numerical cost, being able to treat systems of up to 100 atoms. In the LDA+GdW approximation the quasiparticle self-energy corrections result from the difference between the correct semiconducting screening and hypothetical metallic screening.

Our results show how the optical properties of TMDCs are modified in different situations, e.g. when the screening of the substrate is taken into account, in the presence of vacancies, or when three excited particles form a correlated trion state.

[1] M. Rohlfing, Phys. Rev. B. **82**, 205127 (2010)

TT 71.5 Thu 11:45 S054

Scanning tunneling light emission from single layer MoS_2 — •Christian Lotze, Nils Krane, Julia Läger, Gaël Reecht, and Katharina J. Franke — FU Berlin, FB Physik, Arnimallee 14, 14195 Berlin

Transition-metal dichalcogenides form a group of interesting 2d materials. Among them, the semiconductor MoS_2 has attracted great interest, because it has been shown that it turns from an indirect-gap into a direct-gap semiconductor when reduced to a single layer [1]. As such, potential applications involve its usage for instance as light emitting device.

Here, we present a combined low temperature scanning tunneling (STM) and light emission (LE) study on MoS_2/Au(111). The STM geometry allows to locally inject electrons or holes with the tip into the single layer MoS_2. Inelastically tunneling electrons and holes can give rise to emission of photons [2,3]. Here, we detect and analyze spectrally resolved the electroluminescence from the MoS_2 monolayer on Au(111). We correlate these LE spectra with the electronic structure, that we obtained from scanning tunneling spectroscopy. Moreover we will look into the spatial variation of the LE signals and the role of defect sites.

[1] Mak *et al.*, PRL 105, 136805 (2010)
[2] Berndt *et al.*, PRL 67, 3796 (1991)
[3] Hoffmann *et al.*, Phys. Rev. Lett. 93, 076102 (2004)

TT 71.6 Thu 12:00 S054

Ultrafast photocurrent dynamics in monolayer MoS2 — Eric Parzinger, Anna Vernickel, Alexander Holleitner, and •Ursula Wurstbauer — Walter Schotty Institut and Physik Department, Technical University of Munich, Germany

Atomically thin semiconducting transition metal dichalcogenides such as MoS_2 are emergent materials for optical and electronic circuits. For possible high-frequency applications, we investigate the ultrafast photocurrents in monolayer MoS_2 on a picosecond time scale utilizing a recently developed pump-probe spectroscopy [1-3]. The observed photocurrent contains three major contributions [4]. An initial ultrafast response of $\leq$ 5ps is followed by an exponential decay within a few hundreds of picoseconds. The third very slow contribution peaks at around 1.5 ns. This slow part dominates the overall time-integrated photocurrent intensity. We discuss the impact of laser-induced heating, the one of built-in fields at metal contacts, and the role of trap states. We acknowledge the financial support by the ERC-grant NanoREAL, the DFG excellence cluster Nanosystems Initiative Munich (NIM), and BaCaTec. [1] L. Prechtel, et al. Nature Communications 3, 646 (2012). [2] A. Brenneis, et al. Nature Nanotechnology 10, 135 (2015). [3] C. Kastl, et al. Nature Communications 6, 6617 (2015). [4] E. Parzinger et al. (2016).

TT 71.7 Thu 12:15 S054

Electronic excitations in transition metal dichalcogenides under the influence of dielectric environments — •Malte Rösner[1], Alexander Steinhoff[2], Roelof Groenewald[3], Frank Jahnke[2], Stephan Haas[3], Christopher Gies[2], and Tim O. Wehling[1] — [1]Institut für Theoretische Physik and Bremen Center for Computational Materials Science, Universität Bremen, Bremen, Germany — [2]Institut für Theoretische Physik, Universität Bremen, Bremen, Germany — [3]Department of Physics and Astronomy, University of Southern California, Los Angeles, CA, USA

We present a material-realistic approach to describe electronic interaction effects in transition metal dichalcogenides. On the basis of the Wannier function continuum electrostatics (WFCE) method [1], we are able to include the effects of the dielectric environment, which could serve as a promising tuning knob to control 2D material's properties. We study the doping dependence and the influence of different types of dielectric environments to electronic and plasmonic properties. We find electronic band structure and plasmon dispersion changes on the eV scale.

[1] M. Rösner et al., Phys. Rev. B 92, 085102 (2015)

TT 71.8 Thu 12:30 S054

Optoelectronic properties of sub-nanometer WS2 and TiS3 investigated by scanning near-field optical microscopy and nano-FTIR spectroscopy by using synchrotron radiation — •P. Patoka[1], G. Ulrich[1], A. Nguyen[2], A. Lipatov[3], A. Sinitskii[3], P. Hermann[4], B. Kästner[4], A. Hoehl[4], L. Bartels[2], P. Dowben[5], G. Ulm[4], and E. Rühl[1] — [1]Physikalische Chemie, Freie Universität Berlin, Germany — [2]Dept. of Chemistry, Univ. of California Riverside, U.S.A. — [3]Dept. of Chemistry, Univ. of Nebraska-Lincoln, U.S.A. — [4]Physikalisch-Technische Bundesanstalt (PTB), Germany — [5]Dept. of Physics and Astronomy, Univ. of Nebraska-Lincoln, U.S.A.

Among the 2D electronic materials that have received increased attention recently are the transition metal dichalcogenides (TMD). These materials, especially below nanometer thickness, exhibit promising optoelectronic properties for applications in low-dimension electronic circuits. The combined use of scattering-type near-field optical microscopy and the broadband synchrotron radiation source MLS (PTB, Berlin) allows for the highly sensitive spectromicroscopic characterization of such 2D semiconductors with a spatial resolution below 30 nm. We will present recent results on near-field imaging and nano-FTIR spectroscopy in mid-infrared regime down to monolayer thick TMD structures. Investigated are optical responses of WS2, such as its interaction with the optical phonon mode of the SiO2 substrate. We will also show evidence for high charge accumulation at the edges of the TiS3 structures revealed by optical mapping using tunable CO2 laser.

TT 71.9 Thu 12:45 S054

Investigations on the Phonon Spectrum of $TiSe_2$ in the CDW Phase — •Roland Hott, Rolf Heid, and Frank Weber — Karlsruhe Institute of Technology, Institute of Solid State Physics, P.O.B. 3640, D-76021 Karlsruhe, Germany

We report recent results of our investigations on the Charge Density Wave (CDW) phase transition in $TiSe_2$, performed both experimentally by means of high resolution Inelastic X-ray Scattering (IXS) as well as theoretically by Density Functional Theory (DFT) based ab-initio phonon calculations [1].

We extended our calculations to the case of Cu-doping where we found a huge hardening of the CDW-related soft phonon due to strong chemical bonding of the Cu atoms to the $TiSe_2$ host lattice. Moreover, we investigated the phonon spectrum of $TiSe_2$ in the CDW phase where we find the expected stabilisation of the lattice. Nevertheless, we still obtain here a sizeable electron-phonon coupling for the phonons which derive from the soft phonons of the normal (CDW-undistorted) phase.

[1] F. Weber, S. Rosenkranz, J.-P. Castellan, R. Osborn, G. Karapetrov, R. Hott, R. Heid, K.-P. Bohnen, A. Alatas, PRL **107**, 266401 (2011)

TT 71.10 Thu 13:00 S054

Ultrafast carrier multiplication in 1T-$TiSe_2$ — •Stephan Michael[1], Steffen Eich[1], Henry C. Kapteyn[2], Margaret M. Murnane[2], Michael Bauer[3], Kai Rossnagel[3], Hans Christian Schneider[1], Martin Aeschlimann[1], and Stefan Mathias[4] — [1]University of Kaiserslautern — [2]JILA, University of Colorado and NIST — [3]University of Kiel — [4]University of Göttingen

1T-$TiSe_2$ is a transition metal dichalcogenide, which has a charge density wave (CDW) state below a temperature of around 200 K, which may be due to an excitonic insulator mechanism and/or an Jahn-

Teller effect. We studied optically excited carrier dynamics on ultrashort timescales in the CDW phase using time-resolved ARPES measurements and an effective two-band model including carrier-carrier Coulomb scattering. In the framework of this model we analyze the ultrafast response of this material to optical excitation, which is seen in the experiment. We show that carrier multiplication in the form of impact ionization is the most satisfactory explanation for the ultrafast redistribution of spectral weight observed in the ARPES measurements.

TT 71.11 Thu 13:15 S054

Charge density wave kinetics in 1T-TaS_2 monitored by ultrafast LEED — •Simon Schweda[1], Gero Storeck[1], Sebastian Schramm[1], Max Gulde[1], Kai Rossnagel[2], Sascha Schäfer[1], and Claus Ropers[1] — [1]IV. Physikalisches Institut, Universität Göttingen, D-37077 Göttingen — [2]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel

We developed an ultrafast low-energy electron diffraction (ULEED) setup for the study of time-resolved structural dynamics at surfaces, extending our previous approach operating on ultrathin films in transmission [1]. A laser-driven nanometric needle emitter provides well-collimated electron pulses with durations of few tens of ps at the sample for electron energies in the range of 50-200 eV.

In a first application of this technique, we investigate optically induced transitions between charge density wave (CDW) phases [2] at a single-crystalline 1T-TaS_2 surface. In particular, the recovery of the nearly commensurate (NC) room-temperature phase after laser-excitation to the incommensurate (IC) phase is resolved in the time-domain. We find a strong dependence of the formation time on the energy density deposited. Furthermore, at higher optical fluences, the appearance of metastable NC antiphase domains is observed, caused by a rapid quench after optical excitation. Our results demonstrate the potential of ULEED for the study of complex ultrafast structural and electronic processes at surfaces.

[1] M. Gulde et al., Science 345, 200 (2014)
[2] M. Eichberger et al., Nature 468, 799 (2010)

TT 72: Topological Insulators I (Joint session of DS, HL, MA, O and TT organized by HL)

Time: Thursday 14:45–17:15 Location: H10

TT 72.1 Thu 14:45 H10

Topological Dirac Semimetal in strained HgTe — •Tomáš Rauch[1], Steven Achilles[1], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle (Saale), Germany

HgTe, one of the most intensively investigated materials in the context of topological insulators, is a semimetal with zero energy band gap when considered as a three-dimensional material. Applying uniaxial strain in [001] direction changes the situation dramatically [1]. Under compressive strain HgTe becomes a strong topological insulator featuring typical Dirac cone shaped surface states at the $\overline{\Gamma}$ point of the surface Brillouin zone. On the other hand, applying a tensile strain makes HgTe a topological Dirac semimetal with a pair of doubly-degenerate Dirac cones located along the k_z axis of the bulk Brillouin zone.

By combined *ab initio* and tight-binding electronic structure calculations we investigate the bulk and surface electronic properties of three-dimensional HgTe in the topological Dirac semimetal phase. This includes calculating the bulk band structure, topological invariants, and the electronic structure of the (100) surface, at which the associated non-trivial surface states emerge.

[1] T. Rauch *et al.*, Phys. Rev. Lett. **114**, 236805 (2015)

TT 72.2 Thu 15:00 H10

Tight-Binding Approach towards an Effective Model for InAs/GaSb Quantum Wells — •Matthias Sitte[1], Karin Everschor-Sitte[1], and Allan MacDonald[2] — [1]Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudingerweg 7, 55128 Mainz — [2]The University of Texas at Austin, Department of Physics, 2515 Speedway, Austin, TX 78712-1192

Topological insulators have attracted a great deal of attention as a new quantum state of matter in the last decade. The first realizations of 2D TIs were HgTe/CdTe quantum well heterostructures, but in recent years another class of semiconductor heterostructures — namely InAs/GaSb quantum wells — was shown to yield 2D TIs as well. Compared to the HgTe/CdTe-based systems they have many advantages, most prominently a continuously tunable band structure via external electric fields and stronger proximity coupling to superconductors. We perform empirical tight-binding calculations on these systems to study how topological properties are changed by varying external control parameters such as electric fields or well thicknesses.

TT 72.3 Thu 15:15 H10

Negative Magnetoresistance of $TlBi_xSb_{1-x}Te_2$ — •Oliver Breunig, Zhiwei Wang, Fan Yang, Alexey Taskin, and Yoichi Ando — II. Physikalisches Institut, Universität zu Köln

In the family of the ternary II-V-VI_2 compounds several materials have been identified as topological insulators. In the n-type $TlBiTe_2$ a topological surface state has been found, yet it is hardly accessible for transport studies due to the overlap with the bulk bands. Theoretical studies suggest that upon substituting Bi by Sb a narrow bulk band gap opens while preserving a single Dirac cone at the Γ point, leading to a possible realization of a bulk-insulating system with an exposed Dirac point.

Single crystals of $TlBi_xSb_{1-x}Te_2$ were grown by a modified Bridgman technique using high-purity starting materials. They were characterized by ICP/EDX as well as transport measurements. For intermediate values x we find insulating transport properties and a surprisingly strong negative magnetoresistance. We present our crystal growth results of $TlBi_xSb_{1-x}Te_2$ and discuss the origin of the observed large negative magnetoresistance.

TT 72.4 Thu 15:30 H10

Landau level spectroscopy of the 3D topological insulator Sb_2Te_3 — •Stefan Wilfert[1], Oliver Storz[1], Paolo Sessi[1], Thomas Bathon[1], Konstantin Kokh[2], Oleg Evgen'evich Tereshchenko[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Novosibirsk State University, 630090 Novosibirsk, Russia

Sb_2Te_3 is a prototypical three-dimensional topological insulator (TI) with intrinsic p-doping, which leads to a Dirac point lying well above the Fermi level [1]. We performed energy-dependent quasi-particle interference mapping and scanning tunnel spectroscopy in high magnetic fields up to 12 T on this compound, where both methods allow to obtain the energy dispersion. In contrast to the much more studied TIs Bi_2Te_3 [2] and Bi_2Se_3 [3], Sb_2Te_3 shows Landau levels with both negative and positive Landau level indices. This enables to analyze in more detail the energetic broadening of the Landau levels, which may lead to a better understanding of the physical limits of quantum coherence in this type of materials.

[1] C. Seibel *et al.*, Phys. Rev. Lett. **114**, 066802 (2015).
[2] Y. Okada *et al.*, Phys. Rev. Lett. **109**, 166407 (2012).
[3] T. Hanaguri *et al.*, Phys. Rev. B **82**, 081305 (2015).

30 min. Coffee Break

TT 72.5 Thu 16:15 H10

Aharonov-Bohm effect in the 3D topological insulator HgTe — •Johannes Ziegler[1], Dmitriy Kozlov[1,2,3], Dmitry Kvon[2,3], Nikolay Mikhailov[2], Sergey Dvoretsky[2], and Dieter Weiss[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]A.V. Rzhanov Institue of Semiconductor Physics, Novosibirsk, Russia — [3]Novosibirsk State University, Russia

We present our progress in the investigation of the Aharonov-Bohm effect in ring and nanowire structures, fabricated from high-mobility strained 80 nm HgTe films with a wet etching technique. The nanostructures are equipped with topgates to allow tuning of the Fermi level E_f and are measured in a dilution cryostat.

The focus lies on Topological Insulator nanowires, where it is expected that the magnetic flux Φ through the wire leads to both Φ_0 and $\Phi_0/2$ periodic oscillations [1]. Φ_0 $(= h/e)$ periodic oscillations are expected to occur in the ballistic regime for a large range in E_f. For ballistic devices, both minima and maxima of the conductance are expected at $\Phi = \Phi_0/2$ with varying E_f. In the case of diffusive transport, Φ_0 periodic oscillations are expected for E_f close to the Dirac point, while tuning E_f away from the Dirac Point leads to $\Phi_0/2$ $(= h/2e)$ periodic oscillations.

[1] J.H. Bardarson *et al.*, Phys. Rev. L **105**, 156803 (2010)

TT 72.6 Thu 16:30 H10

Emergence of quantum spin Hall and half-topological states at Graphene/TMDC heterostructures — •Denis Kochan, Martin Gmitra, Petra Högl, and Jaroslav Fabian — Institute for Theoretical Physics, University of Regensburg, Germany

We discuss orbital and spin-orbital proximity effects emerging in graphene deposited on a monolayer transition-metal dichalcogenides (TMDCs: MoS2, MoSe2, WS2, WSe2) and analyze the impact on spin transport in such graphene/TMDC heterostructures. First-principles investigations show that graphene on MoS2, MoSe2, and WS2 has a topologically trivial band structure, while graphene on WSe2 exhibits inverted bands. The essential low energy physics can be well described by a symmetry inspired realistic tight-binding Hamiltonian. We predict topologically protected helical edge states for graphene zigzag nanoribbons on WSe2, demonstrating the emergence of the quantum spin Hall effect. Our model also features "half- topological states", which are protected against time-reversal disorder on one edge only. Unlike in pristine graphene, the proximity spin-orbit coupling in graphene on TMDCs is significant (orders of meV), making the predicted effect testable experimentally.

This research was supported by DFG SFB 689, GRK 1570 and by the EU Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

TT 72.7 Thu 16:45 H10

Chiral Magnetic Effect in an Interacting Weyl Semimetal — •Matthias Puhr, Semen Valgushev, and Pavel Buividovich — Universität Regensburg, D-93053 Regensburg, Deutschland

We present results of a mean-field study of the chiral magnetic effect in a simple model of a parity-breaking Weyl semimetal. Our model is given by the lattice Wilson-Dirac Hamiltonian with on-site repulsive interaction and a constant chiral chemical potential term. We find a non-trivial behaviour of the chiral magnetic conductivity (CMC) and observe an increase, a decrease and even a change of sign depending on the interaction strength. The absolute value of the CMC never exceeds the value for the non-interacting gapless Hamiltonian. Our model exhibits a phase transition to a phase with spontaneously broken parity (Aoki phase, axionic insulator phase) and we observe a strong suppression of the CMC in the parity broken phase.

TT 72.8 Thu 17:00 H10

Negative magneto-resistivity in finite-size samples of Weyl semimetals — Pavel Buividovich, Matthias Puhr, and •Semen Valgushev — University of Regensburg, Regensburg, Germany

We numerically study Chiral Magnetic Effect and magneto-resistivity in a slab of parity-breaking Weyl semimetal modeled by Wilson-Dirac hamiltonian with open boundary conditions and subjected to the external magnetic field parallel to the boundaries. We find that the density of CME current is locally non-zero and strongly localized near the boundaries, where it approaches conventional value $j = \mu_5 B/2\pi^2$. We calculate the magneto-resistivity in a physical setup when parallel magnetic and electric fields are applied to the sample and discuss our results in the context of recent experiments on negative magneto-resistivity in Weyl semimetals.

TT 73: Low-Dimensional Systems: Topological Order

Time: Thursday 15:00–18:00 Location: H19

TT 73.1 Thu 15:00 H19

Trivial and topological phases protected by symmetries in spin-2 quantum chains — •Augustine Kshetrimayum[1], Hong-Hao Tu[2], and Román Orús[1] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

Symmetry-protected trivial (SPt) phases of matter are the product-state analogue of symmetry-protected topological (SPT) phases. This means, SPt phases can be adiabatically connected to a product state by some path that preserves the protecting symmetry. Moreover, SPt and SPT phases can be adiabatically connected to each other when interaction terms that break the symmetries protecting the SPT order are added in the Hamiltonian. It is also known that spin-1 SPT phases in quantum spin chains can emerge as effective intermediate phases of spin-2 Hamiltonians. In this talk, we show that a similar scenario is also valid for SPt phases. More precisely, we show that for a given spin-2 quantum chain, effective intermediate spin-1 SPt phases emerge in some regions of the phase diagram, these also being adiabatically connected to non-trivial intermediate SPT phases. We characterize the phase diagram of our model by studying quantities such as the entanglement entropy, symmetry-related order parameters, and 1-site fidelities. Moreover, we provide a field theory description of the quantum phase transitions between the SPt phases.

TT 73.2 Thu 15:15 H19

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 different vortex sectors. 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 73.3 Thu 15:30 H19

Projective construction of the Zk Read-Rezayi fractional quantum Hall states and their excitations on the torus geometry — •Cecile Repellin[1,2], Titus Neupert[3], B. Andrei Bernevig[4], and Nicolas Regnault[2,4] — [1]Max-Planck-Institut fur Physik complexer Systeme, Dresden, Germany — [2]Laboratoire Pierre Aigrain, Ecole Normale Superieure, Paris, France — [3]Princeton Center for Theoretical Science, Princeton, USA — [4]Princeton University, Princeton, USA

Multilayer fractional quantum Hall wave functions can be used to construct the non-Abelian states of the Zk Read-Rezayi series upon symmetrization over the layer index. Unfortunately, this construction does not yield the complete set of Zk ground states on the torus. We develop an alternative projective construction of Zk Read-Rezayi states that complements the existing one. On the multi-layer torus geometry, our construction consists of introducing twisted boundary conditions connecting the layers before performing the symmetrization. We give a comprehensive account of this construction for bosonic states, and numerically show that the full ground state and quasihole manifolds are recovered for all computationally accessible system sizes. Furthermore, we analyze the neutral excitation modes above the Moore-Read on the torus through an extensive exact diagonalization study. We show numerically that our construction can be used to obtain excellent approximations to these modes. Finally, we extend the new symmetrization scheme to the plane and sphere geometries.

TT 73.4 Thu 15:45 H19

Density matrix renormalization group on a cylinder in mixed real and momentum space — •Johannes Motruk[1], Michael P. Zaletel[2], Roger S. K. Mong[3], and Frank Pollmann[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Station Q, Microsoft Research, Santa

Barbara, CA 93106, USA — [3]Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, USA

We present a variant of the density matrix renormalization group (DMRG) algorithm for two-dimensional cylinders that uses a real space representation along the cylinder and a momentum space representation in the perpendicular direction. This mixed approach allows us to use the momentum around the circumference as a conserved quantity in the DMRG algorithm which greatly reduces computational costs compared to the traditional purely real space approach. Applying the method to the interacting fermionic Hofstadter model at integer and fractional fillings, we demonstrate a considerable speedup in computation time and a substantial reduction of memory usage.

TT 73.5 Thu 16:00 H19

Topological edge states in a one-dimensional ladder system — •Kai-Simon Guther, Nicolai Lang, and Hans Peter Büchler — Institut für Theoretische Physik III, Universität Stuttgart

We consider an interacting, particle number conserving model of fermions in a two-wire system. An exact solution for the ground state is possible for a special choice of parameters, and the occurence of topological edge states with non-Abelian statistics has been proven previously analytically [1].

We analyze the stability of the edge states and the corresponding ground state degeneracy away from the exactly solvable point. Therefore, we empoly both a perturbative approach using bosonization as well as the numerical method of density matrix renormalization group. We demonstrate the stability of the edge state under certain perturbations while other perturbations lead to the occurence of a phase separation. We derive the phase diagram in which the exactly solvable point is located at a phase boundary similar to that appearing in a model considered in [2].

[1] N. Lang and H. P. Büchler, PRB **92**, 041118 (2015)
[2] F. Iemini et al., PRL **115**, 156402 (2015)

TT 73.6 Thu 16:15 H19

Interaction-driven strong topology on the boundary of a weak topological superconductor — •Daniel Mendler[1,2], Panagiotis Kotetes[1,3], and Gerd Schön[1,2] — [1]Inst. für theo. Festkörperphysik, Karlsruhe Inst. of Technology — [2]Inst. of Nanotechnology, Karlsruhe Inst. of Technology — [3]Center for Quantum Devices, Niels Bohr Inst., U. of Copenhagen

We focus on a class of topological superconductors (TSCs) which exhibit a bulk energy gap and support Majorana flat bands (MFBs) on the surface. In contrast to previous proposals relying on strong TSCs with nodal bandstructure, here MFBs are solely protected by a weak topological invariant reflecting a global or local strong anisotropy. In the present case interactions play a dual role, on one hand driving the spontaneous symmetry breaking to an anisotropic superconducting phase and on the other, gapping out the arising MFBs yielding a strong topological phase on the boundary. The prototype system showing this kind of behavior is the nematic p_z-superconductor, which supports surface MFBs. While the interactions stabilize the p_z-SC phase in the bulk and induce the MFBs, suppressed bulk p-wave pairing terms occur on the surface, thus lifting the MFB-degeneracy. A similar situation can take place if the nematic features are only local, a scenario which is realizable in a heterostructure consisting of a conventional superconductor in proximity to a topological insulator surface with intrinsic magnetic order.

15 min. break

Invited Talk TT 73.7 Thu 16:45 H19

Imaging currents in 2D quantum materials — •Katja Nowack — Cornell University, Ithaca, United States

Magnetic imaging is uniquely suited to the non-invasive imaging of current densities, particularly in 2D devices. In this talk, I will showcase this approach by discussing our measurements on HgTe quantum well devices in the quantum spin Hall (QSH) regime. In a nutshell, we scan a superconducting quantum interference device (SQUID) to obtain maps of the magnetic field produced by the current flowing in a device. From the magnetic image we reconstruct a 2D current distribution with a spatial resolution of several microns. This allowed us to directly visualize that the edges of the devices carry most of the current when tuned into their insulating gaps - a key feature of the QSH state. In addition, from the images we disentangle conduction through the edges and the interior of a device, allowing us to study the resistance of only the edges even when the interior becomes conductive through either gating or raising the temperature. If time permits, I will both discuss strategies to improve the spatial resolution of our measurements to sub-micron length scales through a combination of improved image reconstruction and smaller sensor sizes and outline interesting opportunities for current imaging.

TT 73.8 Thu 17:15 H19

Temperature induced crossover in the collision-dominated Dirac semimetal Cd_3As_2 — Azat Sharafeev[1], Vladimir Gnezdilov[1,2], •Peter Lemmens[1], Raman Sankar[3], and Fangcheng Chou[3] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE NAS, Ukraine — [3]CCMS, National Taiwan Univ., Taipei, Taiwan

The 3D topological Dirac semimetal Cd_3As_2 was studied in a wide range of temperatures and excitation energies using Raman spectroscopy. The temperature evolution of the phononic and the quasielastic electronic scattering is discussed in terms of a collision-dominated regime with pronounced electronic energy density fluctuations. A crossover is observed in the intensity of the signals attributed to a collision-dominated phonon regime.

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

TT 73.9 Thu 17:30 H19

Magnetic behaviour of the honeycomb antiferromagnet $BaNi_2V_2O_8$ — •Ekaterina Klyushina[1,2], Bella Lake[1,2], Nazmul Islam[1], Bastian Klemke[1], Astrid Schneidewind[3], Jitae Park[3], and Martin Mansson[4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [3]Heinz Maier-Leibnitz Zentrum, TU München, Garching, Germany — [4]Paul Scherrer Institute, Switzerland

Here we present our recent investigations of a spin-1 honeycomb antiferromagnetic $BaNi_2V_2O_8$ which is a highly 2D antiferromagnet with XY anisotropy making this compound a potential candidate for the Berezinsky-Kosterliz-Thouless topological phase transition [1,2]. Single crystal inelastic neutron scattering measurements in the honeycomb plane at 4 K reveal that the magnetic excitations extend from 0.3-26 meV and consist of two anisotropy-split gapped modes with gaps of 0.3 meV and 3.3 meV arising from the anisotropy within the a-b plane and XY anisotropy respectively . The excitations agree well with simulations based on linear spin - wave theory and are completely dispersionless in the out-of-plane direction suggesting negligible interplane coupling in spite of the long range magnetic order below $T_N = 48$ K. A detailed investigation of the order parameter and correlation length are presented and compared to various theories.

[1] J. M. Kosterlitz, D. J. Thouless J. Phys. C **6**, 1181 (1973)
[2] A. Cuccoli et al., PRB **67**, 104414 (2003)

TT 73.10 Thu 17:45 H19

Nonabelian hierarchies of fractional quantum Hall states — •Yoran Tournois and Maria Hermanns — Institute for Theoretical Physics, Cologne

The fractional quantum Hall effect is one of the paradigmatic examples of topological order in condensed matter physics. It harbors anyonic quasiparticle excitations which carry fractional charge and obey fractional exchange statistics, i.e. when these identical particles are exchanged the wavefunction picks up a complex phase which may take any value between 1 and -1. While the physics of the fractional quantum Hall effect is well understood in the lowest Landau level by means of the Haldane-Halperin hierarchy, this is not the case for the second Landau level. The latter is of particular interest as it is believed that in the second Landau level, even more exotic excitations - nonabelian anyons - may be realized. Several proposals on how to generalize the Haldane-Halperin hierarchy to the second Landau level exist. In this talk, we will consider these different proposals, and discuss how to obtain the properties of their nonabelian excitations.

TT 74: Focus Session: Many-Body Interference and Quantum Statistical Physics (Joint session of DY and TT organized by DY)

Fascinating experimental progress in controlling and monitoring quantum many-body systems has triggered broad activities to better understand quantum coherent many-body phenomena, in particular from the perspective of dynamics and many-particle interference in Fock space. In this focus session, both in experimental and theory talks, light is shed on many-particle interference phenomena, for bosonic and fermionic (massive) particles as well as for photons, and their implications for modern quantum statistical physics. [Organizers: Klaus Richter (Universität Regensburg) and Andreas Buchleitner (Universität Freiburg; Chairperson DPG-Section SAMOP)]

Time: Thursday 15:00–17:45 Location: H20

Invited Talk TT 74.1 Thu 15:00 H20

Between Localization and Ergodicity in Quantum Systems — •Boris Altshuler — Columbia University, New York

Strictly speaking the laws of the conventional Statistical Physics, in particular the Equipartition Postulate, apply only in the presence of a thermostat. For a long time this restriction did not look crucial for realistic systems. Recently there appeared two classes of quantum many-body systems with the coupling to the outside world that is (or is hoped to be) negligible: (1) cold quantum gases and (2) systems of qubits, which enjoy a continuous progress in their disentanglement from the environment. To describe such systems properly one should revisit the very foundations of the Statistical Mechanics. The first step in this direction was the development of the concept of Many-Body Localization (MBL) [1]: the states of a many-body system can be localized in the Hilbert space resembling the celebrated Anderson Localization of single particle states in a random potential. Moreover, one-particle localization of the eigenfunctions of the Anderson tight-binding model (on-site disorder) on regular random graphs (RRG) strongly resembles a generic MBL. MBL implies that the state of the system decoupled from the thermostat depends on the initial conditions: the time averaging does not result in equipartition distribution, the entropy never reaches its thermodynamic value i.e. the ergodicity is violated. Variations of e.g. temperature can delocalize many body states. However, the recovery of the equipartition is not likely to follow the delocalization immediately: numerical analysis of the RRG problem suggests that the extended states are multi-fractal at any finite disorder [2]. Moreover, regular (no disorder!) Josephson junction arrays (JJA) under the conditions that are feasible to implement and control experimentally demonstrate both MBL and non-ergodic behavior [3].

[1] D. Basko, I. Aleiner, and B. Altshuler, Ann. Phys. 321, 1126 (2006). [2] A. De Luca, B.L. Altshuler, V.E. Kravtsov, & A. Scardicchio, PRL 113, 046806, (2014) [3] M. Pino, B.L. Altshuler and L.B. Ioffe, arXiv:1501.03853, PNAS to be published.

Invited Talk TT 74.2 Thu 15:30 H20

Canonical description of short-range interacting few-body quantum systems — •Quirin Hummel, Benjamin Geiger, Juan Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

The theoretical study of quantum few-body systems poses a fundamental challenge since the absence of a large number of particles makes the usually simplifying description within the grand canonical formalism invalid. We analytically address the fundamental interplay between indistinguishability, interactions and many-body interference in bosonic and fermionic systems with strictly fixed total particle number; quantum statistics is treated exactly and interparticle forces are described non-perturbatively. We perform calculations for thermodynamic and spectral quantities by expanding the canonical partition function in terms of Ursell operators in the short-time approximation where the discreteness of many-body spectra is neglected. This approach is specially suitable for the few-body case as it generates thermodynamic and spectral properties in terms of a finite set of permutation and interaction events thus overcoming the inappropriate use of virial expansions.

For 1D systems with short-range interactions we present analytical expressions applicable to both integrable prototypical systems such as the Lieb-Liniger and Gaudin-Yang models as well as realistic non-integrable models with harmonic confinement.

Invited Talk TT 74.3 Thu 16:00 H20

One, Two, Three, Many: Manipulating Quantum Systems One Atom at a Time — •Selim Jochim — Physikalisches Institut, Universität Heidelberg, Germany

Experiments with ultracold gases have been extremely successful in studying many body systems, such as Bose Einstein condensates or fermionic superfluids. These are deep in the regime of statistical physics, where adding or removing an individual particle does not matter. For a few-body system this can be dramatically different. This is apparent for example in nuclear physics, where adding a single neutron to a magic nucleus dramatically changes its properties. In our work we deterministically prepare generic model systems containing up to ten ultracold fermionic atoms with tunable short range interaction. In our bottom-up approach, we have started the exploration of such few-body systems with a two-particle system that can be described with an analytic theory. Adding more particles one by one we enter a regime in which an exact theoretical description of the system is exceedingly difficult, until the particle number becomes large enough such that many-body theories provide an adequate approximation.

Our vision is to use our deterministically prepared tunable few-body systems as microscopic building blocks to assemble model systems that might help to gain insight into complex many-body systems.

15 min. break

Invited Talk TT 74.4 Thu 16:45 H20

Statistical Signatures of Many-Particle Interference — •Mattia Walschaers — Physikalisches Institut, Albert-Ludwigs-Universitat Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany — Instituut voor Theoretische Fysica, University of Leuven, Celestijnenlaan 200D, B-3001 Heverlee, Belgium

The complexity of a quantum system drastically increases with the number of its constituents, which gives rise to several difficulties, often associated with the interactions between particles. Nevertheless, already the indistinguishability of particles alone can lead to dynamical interference effects which go well beyond mere quantum statistics, even in the absence of interactions. Recently, these many-particle interferences became the centrepiece of the debate on boson sampling, connecting them to quantum simulation. As a core message, it was explicitly stressed that such interference patterns are computationally intractable. As a consequence, we are confronted with apparent difficulties for the certification of many-particle interferometers. However, from a complex systems perspective, the intractability of the deterministic behaviour of a physical system is common place, and motivates a statistical treatment. In this contribution, we present statistical signatures of different types of many-particle interference by studying correlation functions combined with techniques from random matrix theory [1]. We also show how these signatures are altered by varying the degree of indistinguishability of the particles.

[1] M. Walschaers, J. Kuipers, J.-D. Urbina, K. Mayer, M. C. Tichy, K. Richter, and A. Buchleitner, arXiv:1410.8547 (2014).

Invited Talk TT 74.5 Thu 17:15 H20

Boson sampling with integrated quantum photonics — •Fabio Sciarrino — Dipartimento Sapienza, Università di Roma, Roma, Italy

Boson sampling is a computational task strongly believed to be hard for classical computers, but efficiently solvable by orchestrated bosonic interference in a specialized quantum computer. Current experimental schemes, however, are still insufficient for a convincing demonstration of the advantage of quantum over classical computation. A new variation of this task, scattershot boson sampling, leads to an exponential increase in speed of the quantum device, using a larger number of photon sources based on parametric down-conversion. This is achieved

by having multiple heralded single photons being sent, shot by shot, into different random input ports of the interferometer. We report the first scattershot boson sampling experiments, where six different photon-pair sources are coupled to integrated photonic circuits. We use recently proposed statistical tools to analyze our experimental data, providing strong evidence that our photonic quantum simulator works as expected. This approach represents an important leap toward a convincing experimental demonstration of the quantum computational supremacy.

TT 75: Transport: Molecular Electronics and Photonics 2 (Joint session of CPP, DS, HL, MA, O and TT organized by TT)

Time: Thursday 15:00–16:00 Location: H23

TT 75.1 Thu 15:00 H23

First-principles calculation of the thermoelectric figure of merit for [2,2]paracyclophane-based single-molecule junctions — •Marius Buerkle[1], Fabian Pauly[2], and Yoshihiro Asai[1] — [1]AIST Tsukuba — [2]University Konstanz

Here we present a theoretical study of the thermoelectric transport through [2,2]paracyclophane-based single-molecule junctions [1]. Combining electronic and vibrational structures, obtained from density functional theory (DFT), with nonequilibrium Green's function techniques allows us to treat both electronic and phononic transport properties at a first-principles level. Paracyclophane derivatives offer a great flexibility in tuning their chemical properties by attaching different functional groups. We show that, for the specific molecule, the functional groups mainly influence the thermopower, allowing us to tune its sign and absolute value. We predict that the functionalization of the bare paracyclophane leads to a largely enhanced electronic contribution ZelT to the figure of merit. Nevertheless, the high phononic contribution to the thermal conductance strongly suppresses ZT. Our work demonstrates the importance to include the phonon thermal conductance for any realistic estimate of the ZT for off-resonant molecular transport junctions.

[1] M. Buerkle et al., PRB **91**, 165419 (2015)

TT 75.2 Thu 15:15 H23

Switching the conductance of a molecular junction by proton transfer — •Dominik Weckbecker, Pedro B. Coto, Chriszandro Hofmeister, and Michael Thoss — Institut für Theoretische Physik, Staudtstraße 7/B2, 91058 Erlangen, Germany

The idea of designing switches or diodes using single molecules has motivated intensive experimental and theoretical research on the conductance properties of these systems. In particular, it has been demonstrated that a molecular junction may be used as a nanoswitch if the molecular bridge has two stable states with different conductance that can be reversibly transformed into each other [1]. In this contribution, we explore the possibility of switching a molecular junction using a proton transfer reaction triggered by an external electrostatic field [2]. The study uses transport theory based on first-principles electronic structure calculations [2,3] and considers molecular junctions with graphene or gold as material for electrodes. We show that for the systems investigated, proton transfer can be used for the reversible interconversion between two states, which exhibit different degrees of delocalization of the π-electrons and therefore very different conductance.

[1] S. J. van der Molen et al., J. Phys.: Cond. Mat. **22**, 133001 (2010)
[2] C. Hofmeister et al., J. Mol. Model. **20**, 2163 (2014)
[3] M. Brandbyge et al., PRB **65**, 165401 (2002)

TT 75.3 Thu 15:30 H23

Design rules for molecular electronics: Diarylethene molecules und derivatives — •Lokamani Lokamani[1], Torsten Sendler[1], Peter Zahn[1], Sibylle Gemming[1,2], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01314 Dresden, Germany. — [2]Instiute 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[1] 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. In addition, these molecules exhibit stable electrical characteristics in both conductance states. Here, we study the electronic transport properties of such derivatives at the level of single molecules. In particular, we analyze the effect of various electron accepting and donating groups on the conductance properties of single molecules attached to gold electrodes. We explore the underlying design rules for molecular electronics comparing break-junction experiments and the theoretical investigations on diarylethene molecules and derivatives.

[1] T. Sendler et al., Advanced Science **2**, 1500017 (2015)

TT 75.4 Thu 15:45 H23

Experimental investigation of the role of electron-phonon-coupling on the Mott critical behavior in the organic charge-transfer salts κ-(BEDT-TTF)$_2$X — •E. Gati[1], M. Garst[2], R.S. Manna[1], U. Tutsch[1], B. Wolf[1], S. Hartmann[1], L. Bartosch[3], T. Sasaki[4], H. Schubert[1], J.A. Schlueter[5], and M. Lang[1] — [1]Physikalisches Inst., Goethe Uni, SFB/TR49, Frankfurt, DE — [2]Inst. f. Theo. Physik, Universität zu Köln, DE — [3]Inst. f. Theo. Physik, Goethe Uni, FfM, DE — [4]IMR, Tohoku University, Sendai, Japan — [5]Materials Science Division, Argonne National Laboratory, USA

The Mott transition is one of the key phenomena of strongly correlated electron systems. Of fundamental interest is the determination of its critical behavior and the underlying universality class. Despite intensive experimental efforts, the universality class is still unresolved. A key aspect, which has not been addressed in these approaches, is the role of electron-phonon-coupling as it is supposed to alter the critical properties to Landau criticality [1]. We will present thermal expansion studies under pressure [2] on the organic charger-transfer salt κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl. This technique is a very sensitive tool to detect critical behavior [3] as well as influences of the lattice on the electronic subsystem [1]. Our results clearly show a breakdown of Hooke's law of elasticity which is a direct evidence for significant electron-phonon-coupling. Furthermore, we will discuss its effect on the critical exponents determined by this thermodynamic probe.

[1] Zacharias et al., PRL **109**, 176401 (12)
[2] Manna et al., Rev. Sci. Instrum. **83**, 085111 (2012)
[3] de Souza et al., PRL **99**, 0370031 (2007)

TT 76: Frontiers of Electronic Structure Theory: Focus on Topology and Transport V (Joint session of DS, HL, MA, MM, O and TT organized by O)

Time: Thursday 15:00–18:15 Location: H24

TT 76.1 Thu 15:00 H24

Zero-point renormalization of the electronic structure: trends across chemical and structural space — •Honghui Shang[1], Christian Carbogno[1], Patrick Rinke[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Aalto University, Helsinki, Finland

The importance of the renormalization of the electronic structure due to the zero-point nuclear motion (ZPR) has been discussed since long [1,2], but only recent advances in the first-principles treatment of electron-phonon coupling (EPC) enabled an accurate assessment of this effect for simple, prototypical materials, e.g., diamond [3] and Si [4]. However, it is largely unknown how chemical and structural

properties affect the ZPR. To shed light on this question, we compute the EPC and ZPR for the octet binaries in both the zincblende and NaCl structure. Computationally, this is achieved by exploiting our recent implementation of density-functional perturbation theory in real-space, which provides considerable computational advantages with respect to numerical costs, parallelization, and especially scalability with respect to the number of atoms. We demonstrate the validity of our implementation by comparing with existing studies and finite difference results, investigate the trends across chemical/structural space, and critically discuss the role of the exchange-correlation functional.

[1] P. B. Allen and V. Heine, J. Phys. C **9**, 2305 (1976).
[2] M. Cardona, Solid State Commun. **133**,3 (2005).
[3] F. Giustino,*et.al.* Phys. Rev. Lett. **105**, 265501 (2010).
[4] S. Poncé, *et.al.* J. Chem. Phys. **143**, 102813 (2015).

TT 76.2 Thu 15:15 H24

All-Electron Many-Body Approach to X-Ray Absorption Spectroscopy — •Christian Vorwerk, Caterina Cocchi, and Claudia Draxl — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

We present an all-electron approach of the many-body perturbation theory to describe X-ray absorption spectroscopy (XAS) in solid-state materials. In this formalism, the electron-hole interaction is explicitely included by solving the Bethe-Salpeter equation. A fully relativistic description of core states, as implemented in the all-electron full-potential code `exciting`[1], enables the explicit treatment of the effects of spin-orbit coupling in the spectra. We investigate the XAS for prototypical systems, such as TiO_2 and MgO, considering excitations from oxygen K and metal L edges. Our results, in good agreement with experiments, allow us to gain insight into the nature of the core-level excitations of these materials.

[1] A. Gulans et al., J. Phys. Condens. Matter 26, 363202 (2014).

TT 76.3 Thu 15:30 H24

Cohesive properties from all-electron RPA total energies — •Markus Betzinger[1], Christoph Friedrich[1], Andreas Görling[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

We present an all-electron implementation of the RPA total energy within the full-potential linearized augmented plane-wave (FLAPW) method. An incomplete basis-set correction (IBC) [1] is employed to improve the convergence of the total energy with respect to the basis-set and the number of unoccupied states. To some extent the IBC incorporates an infinite number of bands and enables a virtually exact treatment of the core electrons.
We demonstrate that the core electrons give rise to a sizeable contribution to the RPA total energy. Their individual contribution is comparable to that of the valence electrons. All-electron RPA lattice constants and bulk moduli are shown for a set of prototype materials and compared to experimental results. An excellent agreement with experiment is observed.
[1] M. Betzinger *et al.*, Phys. Rev. B (accepted, 2015); **88**, 075130 (2013); **85**, 245124 (2012).

TT 76.4 Thu 15:45 H24

Explicitly correlated self consistent field theory — •Christian Lasar and Thorsten Klüner — Universität Oldenburg

Explicitly correlated correlation methods are an interesting field of current research since they are able to drastically improve the otherwise slow basis set convergence of conventional correlation methods. Therefore, chemical accuracy can be achieved with rather small basis sets.[1] The new correlation method presented in this contribution has already been developed for two-electron systems a long time ago[2]. We present the generalization of this ansatz to N-electron systems.

The basic idea is to augment a single slater-determinant with an explicitly correlated prefactor which then takes care of the correlation effects and the basis set convergence. Another interpretation of this ansatz would be a contracted CISD with orbital optimization in a complete basis set. The contraction is achieved by the explicitly correlated prefactor whose choice therefore defines the possible accuracy of the method. In principle, the generalization to any pair method i.e. CCSD and MP2 will be possible.

The big advantage of this kind of ansatz for the wave function is the drastic reduction of matrix elements needed for the optimization of the wave function. As a result, the presented method will be applicable to large molecules.

[1] Chem. Rev. 112, p. 4 (2012) [2] J. Chem. Phys. 99, p. 8830 (1993)

TT 76.5 Thu 16:00 H24

Representing energy landscapes by combining neural networks and the empirical valence bond method — •Sinja Klees[1], Ramona Ufer[2], Volodymyr Sergiievskyi[2], Eckhard Spohr[2], and Jörg Behler[1] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Duisburg-Essen, D-45141 Essen, Germany

In recent years, artificial neural networks (NNs) have become a powerful method to develop reactive interatomic potentials for large systems. However, the construction of NN potentials can become computationally very demanding due to the high dimensionality of the configuration space, which needs to be mapped by reference electronic structure calculations. Combining NN potentials with the empirical valence bond (EVB) method offers a promising approach to derive the potential energy of complex systems with substantially reduced effort, since the size of the reference structures can be strongly decreased. Preliminary results will be discussed and compared to density functional theory data.

TT 76.6 Thu 16:15 H24

CELL: a python package for cluster expansions with large parent cells — •Santiago Rigamonti[1], Maria Troppenz[1], Christopher Sutton[2], Luca M. Ghiringhelli[2], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft

The discovery of new materials for applications in areas such as energy harvesting, relies more and more on the accurate theoretical description of complex structures with large unit cells. The properties of interest are often tuned by substitutional dopants. Due to the vast configurational dopant space, a wide-spread approach is the cluster expansion (CE) technique. Most available CE codes are designed for alloys based on small parent cells, with usually 1 to 4 atoms. For the many important materials with much larger parent cells such approaches can't be applied. We devise an iterative scheme, based on efficient samplings of the configurational space, avoiding full structure enumerations. CELL consists of several modules that can be used independently, enabling to design CEs for specific purposes. Various CE schemes are available, offering ℓ_2 and ℓ_1 norms as penalization terms and different cross-validation strategies. Methods such as LASSO and split Bregman iteration are available for dealing with the ℓ_1 norm (compressive sensing). Access to finite-temperature properties and the characterization of phase transitions is possible through the Wang-Landau and diffusive nested sampling modules. Examples are presented for type-I thermoelectric clathrates, with 46 sites in the parent cell.

TT 76.7 Thu 16:30 H24

Structural and electronic properties of the thermoelectric clathrates $Ba_8Al_xSi_{46-x}$ and $Sr_8Al_xSi_{46-x}$ — •Maria Troppenz, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

Clathrate compounds are promising candidates for high-efficiency thermoelectric applications. Their cage-like structure containing guest atoms allows for exploiting the idea of the phonon-glass electron-crystal and reaching a large figure of merit. We study $Ba_8Al_xSi_{46-x}$ and $Sr_8Al_xSi_{46-x}$ ($6 \leq x \leq 16$), where optimal electronic properties are expected close to the Zintl composition ($x = 16$). Cluster expansions on various quantities are performed, thus having access to ground-state as well as finite-temperature properties. A linear increase of the lattice constant with the number of Al substituents is obtained (0.019 Å per Al addition) confirming experimental observations (0.02 Å). The calculated bond distances between high-symmetry sites agree well with experiment for the full compositional range [1,2]. We find a close correlation between bond distances and fractional Al occupancies. This helps improving models used by experimentalists to estimate fractional occupancies. The substitutional configurations present an order-disorder transition around $600 - 900$ K, which is further analyzed applying the Wang-Landau method. An important finding is the semiconducting behavior of the low-temperature ordered phase at the Zintl composition, which points out the technological relevance of these compounds.
[1] J. H. Roudebush *et al.*; *Inorg. Chem.* **51**, 4161 (2012)
[2] M. Bobnar *et al.*; *Dalton Trans.* **44**, 12680 (2015)

TT 76.8 Thu 16:45 H24

***Ab-initio* calculation of Raman spectra of graphene-based materials** — •Albin Hertrich, Caterina Cocchi, Pasquale Pavone, and Claudia Draxl — Department of Physics, Humboldt-Universität zu Berlin, Germany

Raman scattering is an important non-destructive method for characterizing carbon-based materials. The main features of experimental Raman spectra of pristine graphene and graphite are the first-order G-band at ≈1580 cm^{-1} and the dispersive second-order 2D-band at ≈2700 cm^{-1}. We calculate first- and second-order Raman spectra fully *ab-initio* using the full-potential all-electron DFT package `exciting` [1], which allows for the calculation of both phonon dispersion, within the frozen-phonon approximation, and frequency-dependent dielectric tensors, from time-dependent DFT and the Bethe-Salpeter equation. In our approach [2], we expand the dielectric tensor with respect to the phonon normal coordinates. By taking its derivatives and by computing vibrational matrix elements, we calculate Raman scattering intensities. Applying this scheme to monolayer graphene, bilayer graphene, and graphite, we obtain the G-band in good agreement with experiment [3]. Furthermore, we explore the influence of both the stacking sequence and the laser energy on the 2D-band.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[2] C. Ambrosch-Draxl *et al.*, Phys. Rev. B **65**, 064501 (2002).
[3] A. C. Ferrari *et al.*, Phys. Rev. Lett. **97**, 187401 (2006).

TT 76.9 Thu 17:00 H24

Exciton dispersion in layered and 2D systems — •Francesco Sottile[1,2], Giorgia Fugallo[1,2], Pierluigi Cudazzo[1,2], and Matteo Gatti[1,2,3] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-IRAMIS, Université Paris-Saclay, F-91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility — [3]Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, Boîte Postale 48, F-91192 Gif-sur-Yvette, France

The study of the exciton dispersion is of paramount importance for all applications involving light harvesting, beside providing fundamental knowledge about exciton mobility and migration. Using state-of-the-art ab initio many-body approach, like the Bethe-Salpeter equation [1], we present a first principle study of exciton dispersions in layered materials and 2D systems. Results for the former systems (on the prototypical hBN and MoS2) have been recently confirmed by experiments carried out at the Synchrotron ESRF [2]. For the latter (2D) systems we investigate exciton dispersion in graphane and hBN. From our results we provide a general picture of the mechanisms governing the dispersion of neutral excitations in 2D systems, and of the role played by the confinement of the electronic charge in setting the exciton binding energy. In particular we found that due to the strongly reduced screening of the Coulomb interaction in low- dimensional materials, the binding energy of both Wannier and Frenkel excitons in the optical spectra is large and comparable in size[3]. [1] M. Gatti et al., Phys. Rev. B 88, 155113 (2013) [2] G. Fugallo et al. Phys. Rev. B 92, 165122 (2015) [3] P. Cudazzo et al. submitted to Phys. Rev. Lett.

TT 76.10 Thu 17:15 H24

Electronic structure of selected superheavy elements (Z>104) — •Hana Cencarikova[1] and Dominik Legut[2] — [1]Institute of Experimental Physics, SAS, Kosice, Slovakia — [2]IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

The electronic structure of selected super-heavy elements (Z>104) have been determined from the first-principle calculations based on the density functional method. To determine the ground-state structure we have calculated number of basic phases including the face-centered cubic, body-centered cubic, simple cubic as well as hexagonal closed packed structures. Our results were obtained using local density approximation for the exchange and correlation effects and without and with the spin-orbit interaction for the band states. The analysis has been focused on the determination of the electronic density of states, electronic band structure dispersion relation, mechanical properties (elastic constants) and selected thermodynamical properties.

TT 76.11 Thu 17:30 H24

Layer-resolved calculated vibrations at gold surfaces — •Andrei Postnikov[1] and Kamil Moldosanov[2] — [1]Université de Lorraine, LCP-A2MC, Metz, France — [2]Kyrgyz-Russian Slavic University, Bishkek, Kyrgyzstan

Vibration modes at (001), (011) and (111) surface of gold are calculated from first principles, using the Siesta method [1] and the frozen phonon approach. Calculations are done on thick slabs of moderate lateral size – (2×2) for (001), (2×3) for (011), (3×3) for (111). This allows to resolve the vibration patterns layer by layer into the depth, in dependence on the in-plane wavevector component, and discriminating the polarisation of vibration modes. One notes the softening of modes at the surface, and an appearance of specifically surfacial modes. The bulk behaviour is largely recovered from the 5th or 6th layer downwards.

This study was driven by an intention to grasp the properties of longitudinal acoustic modes propagating at some depth under the surface of gold nanoparticles, which were an important element of our recent work related to the mechanism of radiofrequency absorption and hence resulting heating of nanoparticles of $\gtrsim 5$ nm size [2]. Since it is difficult to meaningfully incorporate the diversity of the nanoparticles' shapes in a practical calculation, the vibrations beneath the most common facets occurring at the nanoparticles' surface were studied instead.

1. The Siesta method, `http://departments.icmab.es/leem/siesta/` .
2. A. Postnikov and K. Moldosanov, `http://arxiv.org/abs/1508.00735` .

TT 76.12 Thu 17:45 H24

Electronic structure, mechanical and thermodynamic properties of Actinium from first-principles — •Zuzana Grosmanova[1] and Dominik Legut[2] — [1]Nanotechnology, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic — [2]IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

In this work, the mechanical (elastic constants) and thermodynamic properties of actinium were investigated using first-principle calculations. Our results were obtained using density functional theory employing local density and general gradient approximation for the electronic exchange-correlation effects and including the spin-orbit interaction for the band states. The ground-state structure were determined among simple phases like the face-centered cubic, body-centered cubic, simple cubic as well as hexagonal closed packed structures.

TT 76.13 Thu 18:00 H24

Interaction of Tritium and Chlorine 36 with defects in Graphite: Insights from Theory — •Christoph Lechner[1], Philippe Baranek[1], and Holger Vach[2] — [1]EDF Lab Les Renardières, Avenue des Renardieres, F-77818 Moret-sur-Loing Cedex, France — [2]CNRS-LPICM, Ecole Polytechnique, F-91128 Palaiseau Cedex, France

In order to optimize the waste management of nuclear graphite used in power plants, it is important to understand the properties of the activated impurities it contains, such as tritium and chlorine 36. Therefore, a computational study of the interaction of tritium and chlorine 36 with defects in graphite has been achieved at the density functional theory (DFT) level by using the functionals PBE and PBE0 with Grimme's D3 dispersion correction. The physisorption and chemisorption of atomic and molecular hydrogen or chlorine on graphite surfaces, (001), (100), and (110) with or without mono- and divacancies, have been investigated. The stabilities of the formed complexes are interpreted in terms of the formation energy. To obtain insight into the nature of the bonding a population analysis of the systems has been performed. While the bonding of hydrogen is mostly covalent for chemisorption and van der Waals for physisorption, the behavior of chlorine is much more complex. Depending on the defect site, both, dominantly covalent and dominantly charge transfer bonding, is observed. Raman spectra for selected structures have been investigated, in order to evaluate, if the experimentally observed defect bands can be reproduced.

TT 77: Multiferroics
(Joint session of MA, DF, DS, KR and TT organized by MA)

Time: Thursday 15:00–17:30 Location: H34

TT 77.1 Thu 15:00 H34

Skyrmionic and ferromagnetic resonances in magnetoelectric Cu_2OSeO_3 - magnetic vs electric fields — •S. Harms[1], M. Belesi[2], H. Berger[3], J.-F. Ansermet[3], C. Grams[1], P. Becker[1], and J. Hemberger[1] — [1]University of Cologne, Germany — [2]IFW, Dresden, Germany — [3]ICMP, EPFL, Lausanne, Switzerland

Magnetic Skyrmions are topologically stable spin whirls stabilized by spin-orbit interaction in chiral cubic magnets. It has been shown, that skyrmionic structures can be efficiently manipulated by small forces, such as e.g. currents in metallic host materials [1]. It was also shown, that the skyrmion phases in general can be excited by AC magnetic fields in the microwave range. [2].

The magnetoelectric helimagnetic insulator Cu_2OSeO_3 is one of the up to now rare cases of an insulating chiral magnets showing a stable skyrmion lattice embedded in between helical and ferrimagnetic phases. In this compound the lack of magnetic inversion symmetry leads to the occurrence of electric polarization and correspondingly to a magnetoelectric response. We present results of broadband spectroscopy up to 5 GHz trying to disentangle the different influence of electric and magnetic fields.

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

[1] T. Schulz et al., Nature Physics 8, 301-304 (2012).
[2] Y. Onose et al., Phys. Rev. Lett. 109, 037603 (2012).

TT 77.2 Thu 15:15 H34

Multiferroic vs. magnetoelectric properties of the dilution series $[(NH_4)_{1-x}K_x]_2[FeCl_5(H_2O)]$ — •Daniel Brüning[1], Matthias Ackermann[1], Ladislav Bohaty[2], Petra Becker[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Insitut für Kristallographie, Universität zu Köln, Germany

Recently we found that $(NH_4)_2[FeCl_5(H_2O)]$, a member of the antiferromagnetic erythrosiderites $A_2[FeX_5(H_2O)]$ (A = K, Rb, Cs or NH_4 and X = Cl or Br) is multiferroic with a spontaneous polarization at T_C = 6.87K, slightly below the magnetic ordering at T_N = 7.25K. Additionally we found a high-temperature structural phase transition T_{st} = 79K, related to a monoclinic distortion (Pnma to $P11\frac{2}{a}$) due to a rearrangement of the hydrogen atoms. In contrast to $(NH_4)_2[FeCl_5(H_2O)]$, the related erythrosiderites with A = K, Rb or Cs are not multiferroic, but show linear magnetoelectric coupling with $P_i = \alpha_{ij} H_j$ below T_N. Investigating the dilution series with $A = (NH_4)_{1-x}K_x$ provides information on the stability of the multiferroic versus magnetoelectric behavior. Based on dielectric and magnetic measurements we present detailed magnetic-field versus temperature phase diagrams. Interestingly, the mixed crystals develop a finite pyroelectric polarization at T_{st}, whereas there is no indication of pyroelectricity above T_N, neither in the pure (NH_4)-based nor in the pure K-based compound.

M. Ackermann et al., J. Phys.: Condens. Matter, **26**, 506002, (2014)
M. Ackermann et al., New J. Phys., **15** 123001, (2013)

TT 77.3 Thu 15:30 H34

Optical switching of multiferroic domains in $TbMnO_3$ — •Sebastian Manz[1], Masakazu Matsubara[1,2], Jonathan Büchi[1], Thomas Lottermoser[1], Ayato Iyama[3], Tsuyoshi Kimura[3], Dennis Meier[1], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zürich, 8093 Zurich, Switzerland — [2]Department of Physics, Tohoku University, Sendai 980-8578, Japan — [3]Division of Materials Physics, Osaka University, Osaka 560-8531, Japan

Multiferroics with spin-spiral-driven ferroelectricity possess a strong coupling between electric and magnetic domains, rendering them interesting for future technological devices. Controlling these domains on the local scale is an essential prerequisite, e. g. for data storage applications. Current discussions on spin-spiral multiferroics, however, focused on the conversion of one domain state into the other but reversible local manipulation has not been shown yet. As presently demonstrated in ferri- and ferromagnets, all-optical switching offers a promising route to achieve localized control. Here, we demonstrate spatially-resolved optical switching of antiferromagnetism in multiferroic $TbMnO_3$. We manipulate the antiferromagnetic order via the coupled ferroelectric state using a unique relation between the wavelength of the light and the induced polarization change. This allows us to realize reversible switching of multiferroic domains without any external bias fields. To further understand our results, we performed Monte-Carlo simulations which confirmed our findings. Our proof-of-principle experiments show that multiferroic domains and therefore domain walls can be generated and erased entirely optically on the local scale.

TT 77.4 Thu 15:45 H34

Investigation of the photostriction effect in $BiFeO_3$ by means of infrared and optical spectroscopy — •Florian Burkert and Christine Kuntscher — Experimentalphysik II, Universität Augsburg, D-86159 Augsburg, Germany

It has been reported that $BiFeO_3$ crystals change their size during illumination with visible light or ultraviolet radiation [1,2]. We studied the impact of this photostrictive effect on the optical properties of a $BiFeO_3$ single crystal in the infrared up to the ultraviolet frequency range by using an FTIR spectrometer and a CCD spectrograph. During illumination with various radiation sources we observe the appearance of additional absorption features in the optical spectra. We will discuss possible origins of these new features.

[1] B. Kundys et al., Nat. Mater. **9**, 803 (2010)
[2] B. Kundys et al., Phys. Rev. B **85**, 092301 (2012)

15 min. break

TT 77.5 Thu 16:15 H34

Epitaxial engineering of ferrimagnetic $3d$-$5d$ double perovskites as templates for single phase multiferroics — •Vikas Shabadi[1], Ashish Kulkarni[1,2], Philipp Komissinskiy[1], Ivetta Slipukhina[3], Robert Paria Sena[4], Joke Hadermann[4], Rajeev Gupta[2], Hongbin Zhang[1], Marjana Ležaić[3], and Lambert Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, Germany — [2]Materials Science Programme, IIT Kanpur, India — [3]Peter Grünberg Institut, Forschungzentrum Jülich and JARA, Germany — [4]Electron Microscopy for Materials Science (EMAT), University of Antwerp, Belgium

$3d$-$5d$ double perovskites ($A_2BB'O_6$) are of high interest due to the possible large magnetic ordering temperatures [1], multiferroicity, and the influence of spin-orbit coupling. We have for the first time synthesized in thin film form double perovskites with Mn^{2+}/Re^{4+} and Ni^{2+}/Re^{4+} cations at the B/B'-sites and La^{3+} at the A-site, previously predicted by density functional theory (DFT). We have shown the almost perfect ordering at the B-site by X-ray diffraction and high-angle annular dark field scanning transmission electron microscopy. The magnetic properties of the compounds studied by SQUID magnetometry and element specific X-Ray magnetic circular dichroism (XMCD) confirm a robust ferrimagnetic order in agreement with the DFT calculations. The results provide a valuable framework for engineering new single-phase multiferroics with ferroelectrically active A-site cations.

[1] Y. Krockenberger *et al.*, Phys. Rev. B **75**, 020404(R) (2007).

TT 77.6 Thu 16:30 H34

Structural and magnetic properties of orthorombic $ErFeO_3$ from first principles — •Dominik M. Juraschek and Nicola A. Spaldin — Materials Theory, ETH Zürich, Switzerland

We investigate the structural and magnetic properties of orthorhombic $ErFeO_3$ using density functional theory.

Rare-earth orthoferrites ($RFeO_3$) show complex coupled lattice and magnetic properties leading to interesting multifferoic, magnetoelectric and spin-dynamic behaviour.

We find that the PBEsol implementation of the generalized gradient approximation plus Hubbard U (GGA+U) method gives structural properties in good agreement with experiment. Using this approximation, we calculate the lattice dynamical properties, the magnetic ground state and the spin-phonon coupling. Our DFT calculations with erbium's 4f electrons frozen in the pseudopotential cores reproduce the G_x-type antiferromagnetic ordering with weak ferromagnetic

F_z canting that is observed experimentally at high temperatures. This lends support to the proposal that the observed spin reorientation transition at 100 K to a G_z ordering is mediately coupling to erbium's 4f moments.

TT 77.7 Thu 16:45 H34

First-principles calculations on anion doped GaFeO3 — •Jacqueline Atanelov and Peter Mohn — Technische Universität Wien, Institut für Angewandte Physik, Computational Materials Science

We present ab initio DFT calculations performed on stoichiometric and anion doped GaFeO3 substituting O by a C, N and S atom, respectively. Stoichiometric GaFeO3 has an antiferromagnetic (AFM) ground state. The Fe atoms of the sublattices Fe1 and Fe2 couple antiferromagnetically via the O atoms through the superexchange mechanism. Exchanging the for the superexchange important O atom with p-elements of a different valence electron configuration changes the underlying magnetic exchange mechanism and influence the ground state properties which can be used for tuning properties interesting for technical applications. Four different doping configurations were examined revealing a cell site dependent influence on the magnetic properties. Carbon, for example, changes the AFM coupling present in the Fe1-O-Fe2 configuration into a ferrimagnetic exchange for the Fe1-C-Fe2 bond. Depending on the respective cell site C substitution introduces a ferrimagnetic or AFM ground state. Nitrogen alters the ground state magnetic moment as well and Sulfur introduces large structural distortions affecting the, band gap and the overall AFM coupling inside the doped GaFeO3 simulation cell. We give a detailed discussion on the respective magnetic exchange mechanisms and electronic properties with regard to applications as photocatalysis and use the predictive power of ab initio DFT simulations that may trigger future experiments.

TT 77.8 Thu 17:00 H34

Multiferroicity in off-stoichiometric $Ga_xFe_{1-x}O_3$ — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The recently reported observation of room-temperature mutiferroic behavior in $Ga_{0.6}Fe_{1.4}O_3$ (GFO) [1] and ϵ-Fe_2O_3 (eFO) [2] offers new perspectives for electronic devices whose operation is based on the switching of magnetic and electric ferroic ordering, as well as on the strong interaction between the magnetic and ferroelectric order parameters, such as multistate non-volatile memory cells. Unfortunately, the realistic microscopic switching mechanism in still not known for either of these materials. They are isostructural with polar $Pna2_1$ crystalline symmetry. In GFO, disorder in the occupancy of Ga and Fe sites is present, whereas eFO is a fully ordered compound. Their parallel study allows us to understand the influence of disorder on possible ferroelectric properties, and develop criteria to maximize the effect. We will present the results of an evolutionary-algorithm [3] based study of $GaFeO_3$-Fe_2O_3 solid solutions, (i.e., with increasing iron content). We will show the condition at which the proper ferroelectricity arises in GFO multiferroics and characterize the parameters of the ferroelectric phase transition. – We acknowledge financial support by Helmholtz Young Investigators Group Programme VH-NG-409 and through DFG-ANR (GALIMEO Consortium).
[1] A. Thomasson *et al.*, J. Appl. Phys. **113**, 214101 (2013); [2] M. Gich *et al.*, Adv. Mater., **26**, 4645 (2014); [3] http://uspex.stonybrook.edu

TT 77.9 Thu 17:15 H34

Fine-tuning ferroic properties: an X-ray diffraction study of type-II multiferroics — •Yoav William Windsor[1], Mahesh Ramakrishnan[1], Kenta Shimamoto[2], Aurora Alberca[1], Laurenz Rettig[1], Elisabeth Monica Bothschafter[1], Yi Hu[2], Thomas Lippert[2], Christof Schneider[2], and Urs Staub[1] — [1]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [2]General Energy Research Department, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

We present a complete X-ray diffraction study of high-quality crystalline films of a prototypical multiferroic, using soft and hard X-rays. With the prospect of future multiferroic functionalities in mind, we show that epitaxial strain directly controls both of the system's ferroic properties. We demonstrate that strain can be used to "push" the system between different multiferroic phases, and even to fine-tune the magnetic ordering periodicity. We generalize this to show that manipulating the crystal structure by other means allows fine-tuning the ferroic properties in a similar manner.

TT 78: Correlated Electrons: Poster Session

Time: Thursday 15:00–18:30 Location: Poster D

TT 78.1 Thu 15:00 Poster D

CT-QMC-simulations on the single impurity Anderson model with a superconducting bath — •Florian Sohn and Thomas Pruschke — Institut für theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Coupling a heavy fermion impurity to a superconducting lead induces a competition between the Kondo effect and superconductivity in the low temperature regime. This situation has been modeled with a single impurity Anderson model, where the normal state bath is replaced by a BCS-type superconducting bath in mean field approximation. We study this model using a continuous-time quantum Monte Carlo hybridization expansion algorithm. Results include the impurity Green's functions as well as the corresponding spectral functions obtained from analytic continuation. Two side bands are observed which we discuss in the light of Yu-Shiba-Rusinov states [1-3]. We gratefully acknowledge financial support by the DFG project PR293/13-1.
[1] Y. Luh, Acta Phys. Sin. **21**, 75 (1965)
[2] H. Shiba, Prog. Theor. Phys. **40**, 435 (1968)
[3] A. I. Rusinov, Sov. Phys. JETP **29**, 1101 (1969)

TT 78.2 Thu 15:00 Poster D

Dielectric and thermodynamic measurements on the magnetoelectric perovskite $EuTiO_3$ — •Johannes Engelmayer, Christoph Grams, 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 $A = Ba, Pb, Cd$. $BaTiO_3$ is the only ferroelectric alkaline-earth titanate, since ferroelectric long-range order is suppressed in $CaTiO_3$ and $SrTiO_3$ by quantum fluctuations, which is referred to as quantum paraelectric behavior. The rare-earth titanate $EuTiO_3$ is similar to $SrTiO_3$, since it has the same valencies (Eu^{2+},Ti^{4+}) and the same ionic radii. Both are cubic at room temperature and undergo a structural phase transition to tetragonal upon cooling. In contrast to the nonmagnetic Sr^{2+}, the half-filled 4f shell of Eu^{2+} with $S = 7/2$ has a large magnetic moment of $7\mu_B$. Below $T_N = 5.5$ K the localized 4f moments order antiferromagnetically, while rather small fields of 1.5 T are sufficient to saturate the magnetization. Here we present field- and temperature-dependent measurements of magnetization, specific heat, and thermal expansion, exhibiting characteristic anomalies at T_N. Broadband measurements of the permittivity reveal the dynamics of polar domain walls at the onset of the structural phase transition, as well as the materials quantum paraelectric nature that is masked by high conductivity for low frequencies.

This work has been supported by the DFG through the Institutional Strategy of the University of Cologne within the German Excellence Initiative.

TT 78.3 Thu 15:00 Poster D

Low-temperature structure and Fermi surface of (La,Ce)$TiGe_3$ — •Tobias Förster[1], Helge Rosner[2], Jacob Grasemann[1], Marc Uhlarz[1], Wolfram Kittler[3], Veronika Fritsch[4], Oliver Stockert[2], Jochen Wosnitza[1], and Hilbert v. Löhneysen[3] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Max Planck Institute f. Chemical Physics of Solids, Dresden, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany — [4]Institut für Physik, Universität Augsburg, Augsburg, Germany

$CeTiGe_3$ presents the rare case of a ferromagnetically ($T_C \approx 14$ K) ordered Kondo-lattice compound and is probably the first known example of an intermetallic hexagonal perovskite of the $BaNiO_3$ structure type. $LaTiGe_3$ may be used as its nonmagnetic reference, since both

compounds crystallize in the same crystal structure [1,2]. To clarify the interplay between structural, localized, and itinerant degrees of freedom an accurate knowledge of the electronic band structure is necessary. Here, we present a detailed electronic-structure study of both compounds applying full potential density functional calculations. Since the Ge's atomic position couples strongly to the band structure at the Fermi energy, a low-temperature, high-resolution structure refinement was made. We attempt to separate the influence of different parameters on the topology of the respective Fermi surfaces and will compare our results with de Haas-van Alphen measurements.
[1] P. Manfrinetti et al., Solid State Commun. **135** (2005) 444.
[2] W. Kittler et al., PRB **88** (2013) 165123.

TT 78.4 Thu 15:00 Poster D

Thermal transport and thermodynamic properties of the Weyl monophosphide NbP — •Ulrike Stockert, Michael Baenitz, Binghai Yan, Claudia Felser, and Marcus Schmidt — Max Planck Institute for Chemical Physics of Solids, Dresden

NbP is a Weyl semimetal, which exhibits a huge positive magnetoresistance (MR) exceeding 8 x 10^5% at 2 K for an electrical current applied along b and a magnetic field of 9 T along c. The MR is further increasing roughly linearly up to at least 60 T. This finding has been attributed to an ultrahigh charge carrier mobility.

We performed thermal transport and specific heat measurements on NbP for the same configuration, namely the magnetic field B along c and the heat current along b. We find a huge change of the thermopower in magnetic fields with a maximum value of 800 μV/K at 9 T and 50 K. Such large effects have been rarely observed in bulk materials, the only example with a larger magnitude at our knowledge being the doped semiconductor InSb. We suggest that the high charge-carrier mobility held responsible for the giant magnetoresistance of NbP is also causing the large magnetothermopower. In addition, electron-phonon scattering processes may play a role, an idea which is also in line with the observation of quantum oscillations in the thermal conductivity of NbP. These are much larger than expected for the electronic contribution estimated from the Wiedemann-Franz-law. Quantum oscillations are also seen in the thermopower and specific heat data.

TT 78.5 Thu 15:00 Poster D

An integrable $S = \frac{1}{2}$ Heisenberg chain with impurity and modified density of states — •Yahya Öz and Andreas Klümper — Bergische Universität Wuppertal

Starting from the integrable Heisenberg XXZ 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 spinon energy-momentum dispersion for the derivation of the thermodynamic equations of this new model. In these equations, energy e and momentum p take a new dispersion relation of the form $e(p) \simeq p^{\alpha}$ for small momenta where $\alpha < 1$.

TT 78.6 Thu 15:00 Poster D

Quantum criticality gains long-time quantum correlations — •Rouhollah Jafari[1,2] and Alireza Akbari[1] — [1]Asia Pacific Center for Theoretical Physics, Pohang, Gyeongbuk 790-784, Korea — [2]Department of Physics, University of Gothenburg, Sweden

Using the general quantum compass model as an environmental system, the dynamical evolution of the decoherence factors, quantum correlations, and negativity of the central spins has been investigated for different initial states. The relation between the quantum-classical transition of the central system, and the occurrence of an avoided level crossing quantum phase transition in its surrounding system has been analyzed. It is well known that the gapless quantum criticality enhances the decay of decoherence factors[1], while our calculations represent a different story for the gapped critical environment. The results that have been found show that long-time quantum correlations at the critical point are an effect of gapped criticality, and maximum decaying occurs away from the critical point[2].
[1] H. T. Quanet al., PRL **96**, 140604 (2006)
[2] R. Jafari, and A. Akbari, EPL **111**, 10007 (2015)

TT 78.7 Thu 15:00 Poster D

Crystal Growth and Characterization of $CeFe_{1-x}Ru_x$ PO — •Tanita Ballé, Kristin Kliemt, and Cornelius Krellner — Goethe Universität Frankfurt, Kristall- und Materiallabor

CeRuPO is a one of the few heavy fermion systems, which order ferromagnetically at low temperatures (T_C = 15 K), because of dominant RKKY-interaction [1]. CeFePO on the other hand shows no long-range magnetic order even at low temperatures because of dominant Kondo effect [2] (T_K = 10 K). By substituting CeFePO with ruthenium we can reach a quantum critical point, at which the RKKY-interaction and the Kondo effect are equally strong [3]. To study the quantum critical point, and to enlighten the question if the order stays ferromagnetically down to lowest temperatures, high quality crystals are needed. Here, the growth and characterization of the single crystals will be discussed. We obtained mm-sized single crystals of the unsubstituted CeRuPO and CeFePO by a modified Bridgeman method using tin as a flux. The quality of the crystals was verified by Powder-X-Ray-Diffraction, energy dispersive X-ray spectroscopy and Laue backscattering.
[1] C. Krellner et al., PRB **76**, 104418 (2007)
[2] E. M. Brüning et al., PRL **101**, 117206 (2008)
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[3] S. Kitagawa et al., J. Phys. Soc. Jpn. **82**, 033704 (2013)

TT 78.8 Thu 15:00 Poster D

Tuning $ZrFe_4Si_2$ by Ge and Y substitution — •Katharina Weber[1,2], Nandang Mufti[1], Til Goltz[2], Theo Woike[3], Hans-Henning Klauss[2], Christoph Bergmann[1], Helge Rosner[1], and Christoph Geibel[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Institute of Solid State Physics, TU Dresden, Germany — [3]Institute for Structural Physics, TU Dresden, Germany

The intermetallic compound series AFe_4X_2 (A = Y, Lu, Zr; X = Si, Ge) presents a rare case of magnetic frustrated metallic systems. In particular $ZrFe_4Si_2$ is of strong interest because our results indicate this system to be very close to a quantum critical point (QCP) where Fe magnetic order disappears. To get a deeper insight into its ground state, we performed a detailed study of Ge and Y substituted $ZrFe_4Si_2$. The isovalent substitution of Ge for Si induces a negative chemical pressure as Ge is larger than Si. As expected from this, the substitution results in the formation of a well-defined antiferromagnetic order with Néel temperatures increasing up to 25 K at 40 % Ge. This confirms $ZrFe_4Si_2$ to be extremely close to the QCP, just on the magnetic side of it. With the second substitution series $Y_xZr_{1-x}Fe_4Si_2$ we investigate the development from the highly reduced antiferromagnetic order in $ZrFe_4Si_2$ towards the two magnetic transitions at 56 K and 76 K, which we see in YFe_4Si_2.

TT 78.9 Thu 15:00 Poster D

Unusual antiferromagnetic structure of $YbCo_2Si_2$ — N. Mufti[1,2], K. Kaneko[1,3], A. Hoser[4], M. Gutmann[5], C. Geibel[1], C. Krellner[1,6], and •O. Stockert[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden — [2]Department of Physics, State University of Malang, Malang, Indonesia — [3]Quantum Beam Science Center, Japan Atomic Energy Agency, Tokai, Japan — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — [5]ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Didcot, United Kingdom — [6]Physikalisches Institut, Goethe-Universität Frankfurt, Frankfurt

We report on extensive powder and single crystal neutron diffraction experiments to study the magnetic structure in $YbCo_2Si_2$ below the Néel temperature T_N = 1.7 K in detail. Representation analysis has been used to find the possible magnetic structure models compatible with the experiments. Two different magnetically ordered phases can clearly be distinguished. At lowest temperatures a commensurate magnetic structure with a propagation vector $\mathbf{k}_1$ = (0.25 0.25 1) and equal moments or about 1.4 μ_B/Yb is found, while the intermediate phase ($T > 0.9$ K) is characterized by an incommensurate amplitude-modulated magnetic structure with $\mathbf{k}_2$ = (0.25 0.086 1). The magnetic structure in $YbCo_2Si_2$ is in stark contrast to all other compounds of the RCo_2Si_2 family (R = rare earth element) likely due to some itinerancy of the Yb 4f states being responsible for the magnetism.

TT 78.10 Thu 15:00 Poster D

Frustrated magnetism in $Yb_2Fe_{12}P_7$ — •Kai Grube[1], Diego A. Zocco[1], Frank Weber[1], Sebastian Kuntz[1], Ryan Baumbach[2], James Hamlin[3], Ivy Lum[4], Jeff Lynn[5], Qingzhen Huang[5], Marc Janoschek[6], M. Brian Maple[4], and Hilbert von Löhneysen[1] — [1]Karlsruhe Institute of Technology, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]National High Magnetic Field Laboratory, Tallahassee, USA — [3]Departement of Physics, University of Florida, Gainesville, USA — [4]Department of Physics, University of

California, San Diego USA — [5]NIST Center for Neutron Research, Gaithersburg, USA — [6]Los Alamos National Laboratory, USA

$Yb_2Fe_{12}P_7$ is characterized by a low magnetic transition temperature of $T_N \approx 1\,\mathrm{K}$ and the breakdown of Fermi-liquid behavior. These properties suggest the proximity to a quantum critical point (QCP). The non-Fermi-liquid (NFL) behavior, however, does not conform to the standard QCP scenario described by the Hertz-Millis-Moriya theory. We measured thermal expansion, magnetostriction and magnetization. The pressure dependence was studied up to 15 GPa using resistivity measurements in piston cylinder and diamond anvil cells. The measurements reveal that only a small fraction of the Yb moments participate in the long-range magnetic order. The Grüneisen ratio does not diverge for $T \to 0$ indicating that the NFL behavior is not related to a nearby pressure-induced QCP. In view of the unusual noncentrometric crystal structure, our observations might point to geometric frustration of the magnetic moments.

TT 78.11 Thu 15:00 Poster D

Fluctuation dynamics near the quantum critical point in the S=1/2 Ising chain $CoNb_2O_6$ — •Steffen Harms, Johannes Engelmayer, Thomas Lorenz, and Joachim Hemberger — II. Physikalisches Institut, University of Cologne, Germany

$CoNb_2O_6$ is a model system for quantum phase transitions in magnetic field. Its structure consists of layers of CoO_6 octhahedrons separated by non-magnetic NbO_6 layers. The edge-sharing oxygen octahedrons link the Co^{2+}spins via Co-O-Co superexchange and form 1D ferromagnetic zigzag chains along the orthorhombic c axis. Crystal field effects lead to an easy-axis anisotropy of the Co^{2+} moments in the ac plane and to an effective spin-1/2 chain system. The 1D spin system can be described by the Ising model. At T=0K a transverse magnetic field can induce a quantum phase transition from a long range ferromagnetic state into a quantum paramagnetic state. Employing measurements of the complex AC-susceptibility in the frequency range $10\mathrm{MHz} < \nu < 5\mathrm{GHz}$ for temperatures down to 50mK we investigate the slowing down of the magnetic fluctuation dynamics in the vicinity of the critical field at $\mu_0 H$=5.25T [1].

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

[1]: A.W. Kinross et al. PRX **4**, 031008 (2014)

TT 78.12 Thu 15:00 Poster D

Chiral spin-orbital liquids with nodal lines — •Willian Massashi Hisano Natori[1], Rodrigo Gonçalves Pereira[1], and Eduardo Miranda[2] — [1]Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, Brazil — [2]Instituto de Física Gleb Wataghin, Unicamp, Campinas, Brazil

Quantum spin liquids (QSL) are strongly correlated systems that remain magnetically disordered down to 0 K. Although QSLs are known to be the ground state of many model Hamiltonians, their experimental discovery is debated, underlining the importance of research on spin liquid states arising from realistic Hamiltonian models. In this work, we propose a quantum spin-orbital liquid as a stable phase of a spin-orbital model in double ordered perovskites (DOP). This model accounts for antiferromagnetic interactions and strong spin-orbit coupling. We made a global SU(2) and compass symmetries explicit through a convenient representation. Afterwards, we rewrite the Hamiltonian in terms of Majorana fermion operators plus a Z_2 gauge field. A mean-field decoupling preserving the model symmetries was proposed, whose ground state is a QSL characterized by degenerate gapless Fermi lines. The fact that these lines are associated with a topological invariant and the presence of energetically separated surface states indicates that this QSL is topologically non-trivial. Some predicted results are compared with the experimental data available for the spin liquid candidate Ba_2YMoO_6.

TT 78.13 Thu 15:00 Poster D

Thermal Expansion and Magnetostriction Measurements on $PrIr_2Zn_{20}$ — •Andreas Wörl[1], Christian Stingl[1], Akito Sakai[1], Keisuke T. Matsumoto[2], Takahiro Onimaru[2], Toshiro Takabatake[2,3], and Philipp Gegenwart[1] — [1]Experimentalphysics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [2]Graduate School of Advanced Sciences of Matter, Hiroshima University, Higashi-Hiroshima 739-8530, Japan — [3]Institute for Advanced Materials Research, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

Strong hybridization between electric quadrupole moments and conduction electrons gives rise to interesting physical phenomena such as new quantum phases and novel metallic properties. Non-fermi-liquid behavior based on the two channel Kondo effect is predicted by theory. $PrIr_2Zn_{20}$ crystallizes in the $CeCr_2Al_{20}$-type structure, where the Pr^{3+} ions are surrounded by the highly symmetric cubic crystal field of 16 Zn atoms. The ground state is the non-magnetic Γ_3 doublet and carries only electric quadrupole and a magnetic octupole moment. At $T_Q = 0.11\,\mathrm{K}$ the electric quadrupole moments order in a antiferroquadrupolar way. A superconducting transition occurs at $T_c = 0.05\,\mathrm{K}$. The phase transition at $T_Q = 0.11\,\mathrm{K}$ can be suppressed by high magnetic fields parallel to the [100] direction. We investigate the thermal expansion and magnetostriction at low temperatures. By applying high magnetic fields the system is tuned towards a quadrupolar quantum critical point. Furthermore the reaction of the system on breaking the cubic symmetry by compressive stress is explored.

TT 78.14 Thu 15:00 Poster D

Doping studies in hexagonal A_2IrO_3 — •Ina-Marie Pietsch, Friedrich Freund, and Philipp Gegenwart — Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86159 Augsburg, Germany

Hexagonal iridates A_2IrO_3 (A=Na or Li) are spin-orbit Mott insulators and candidate materials for the realization of the highly anisotropic bonding dependent Kitaev magnetic exchange [1]. However, details of the magnetic properties sensitively depend on the balance of various parameters such as bandwidth, Coulomb repulsion, spin-orbit coupling and the trigonal distortion of the IrO_6 octahedron. A partial substitution of Na by smaller Li as well as the partial magnetic depletion for A_2IrO_3 materials provides experimental input on the evolution of magnetic properties [2,3]. Based upon the previous results, a new series of doped A_2IrO_3 materials (including hyperhoneycomb β-Li_2IrO_3 [4]) is synthesized, characterized and magnetically investigated using SQUID magnetometry.

[1] Y. Singh et al., Phys. Rev. Lett. **108**, 127203 (2012).
[2] S. Manni et al., Phys. Rev. B **89**, 241103 (2014).
[3] S. Manni et al., Phys. Rev. B **89**, 241102(R) (2014).
[4] A. Biffin et al., Phys. Rev. B **90**, 205116 (2014).

TT 78.15 Thu 15:00 Poster D

^{7}Li and ^{23}Na NMR measurements on $(Na_{0.75}Li_{0.25})_2IrO_3$ — •Tusharkanti Dey[1], Markus Prinz-Zwick[2], Martina Schädler[2], Friedrich Freund[1], Soham Manni[1], Avinash Mahajan[2,3], Norbert Büttgen[2], and Philipp Gegenwart[1] — [1]EP-VI, Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]EP-V, Electronic Correlations and Magnetism, University of Augsburg, Germany — [3]IIT Bombay, India

An experimental realization of the proposed Kitaev spin-liquid phase in Na_2IrO_3 and Li_2IrO_3 is still a big challenge. Efforts to suppress the magnetic ordering in Na_2IrO_3 by substituting isoelectronic Li in the Na site was partially successful [1, 2]. An earlier report [1] suggests the optimum doping to be 25% where the magnetic ordering is suppressed to 6 K while the structure remains undisturbed. Interestingly, for the $(Na_{0.75}Li_{0.25})_2IrO_3$ sample Na and Li are crystallographically ordered where the Li ions reside at the centre of the Ir honeycombs [1]. We have studied the material using both ^{7}Li and ^{23}Na NMR. Results of our spectra, spin-lattice and spin-spin relaxation measurements will be discussed in the poster.

[1] S. Manni, S. Choi, I. I. Mazin, R. Coldea, M. Altmeyer, H. O. Jeschke, R. Valenti, and P. Gegenwart, Phys. Rev. B **89**, 245113 (2014)
[2] G. Cao, T. F. Qi, L. Li, J. Terzic, V. S. Cao, S. J. Yuan, M. Tovar, G. Murthy, and R. K. Kaul, Phys. Rev. B **88**, 220414(R) (2013)

TT 78.16 Thu 15:00 Poster D

Hints for a pressure-induced phase transition in the honeycomb lattice iridate Na_2IrO_3 probed by infrared microspectroscopy — •Volker Hermann[1], Jihaan Ebad-Allah[1,2], Friedrich Freund[1], Philipp Gegenwart[1], and Christine Kuntscher[1] — [1]Universität Augsburg, 86159 Augsburg, Germany — [2]Department of Physics, University of Tanta, 31527 Tanta, Egypt

Honeycomb lattice iridates A_2IrO_3 with A=Na, Li, Sr,... are discussed in terms of topological insulators and Mott insulators due to their strong spin-orbit coupling [1,2]. Na_2IrO_3 has a layered honeycomb structure with edge-sharing IrO_6 octahedra. We have carried out pressure-dependent reflection and transmission measurements on monocrystalline Na_2IrO_3 in the infrared and visible frequency ranges.

With increasing pressure the phonon modes harden and the Ir 5d crystal field excitations change only slighly. Several observations suggest the occurrence of a pressure-induced phase transition, including splitting and screening of phonon modes.
[1] Ch. H. Kim et al., PRL **108**, 106401 (2012)
[2] Y. Singh and P. Gegenwart, PRB **82**, 064412 (2010)

TT 78.17 Thu 15:00 Poster D

Structural and magnetic properties of $Sr_2Y_{1+x}Ir_{1-x}O_6$ materials — •Gizem Aslan Cansever[1], Maximilian Geyer[1], Christian G.F. Blum[1], Sebastian Gass[1], Kaustuv Manna[3], Franziska Hammerath[1,2], Laura T. Corredor[1], Andrey Maljuk[1], A.U.B. Wolter[1], Sabine Wurmehl[1,2], and Bernd Büchner[1,2] — [1]IFW Dresden, Institute for Solid State Research, 01171 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01062 Dresden, Germany — [3]Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Ir-based materials have attracted a lot of attention because of the competition between the spin-orbit coupling, Coulomb interaction and crystal field [1]. Sr_2YIrO_6 double perovskites with Ir^{+5} ($5d^4$) ions are generally considered to have a nonmagnetic ground state (J=0). However, Sr_2YIrO_6 double perovskites have been reported to exhibit long-range magnetic order at low temperature and the distorted IrO_6 octahedra were discussed to cause the magnetism in this compound [2]. In this study $Sr_2Y_{1+x}Ir_{1-x}O_6$ materials were investigated in relation to structural and magnetic properties with varying Y and Ir concentrations. The samples were prepared by solid-state chemical reaction method. Magnetic susceptibility measurements were performed down to 0.4 K.
[1] G. Khaliullin, PRL **111**, 197201 (2013)
[2] G. Cao et al., PRL **112**, 056402 (2014)

TT 78.18 Thu 15:00 Poster D

High-field multi-frequency ESR spectroscopy of La_2CuIrO_6 — •Stephan Fuchs[1], Vladislav Kataev[1], Kaustuv Manna[1], Sabine Wurmehl[1], Anup Kumar Bera[3], Andrey Malyuk[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 — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

We will present the electron spin resonance results of the double perovskite La_2CuIrO_6. This material provides a playground to examine the magnetic interactions in a 5d transition metal oxide with strong spin-orbit coupling. Measurements of the static magnetization M(T,H) show an antiferromagnetic ordering at $T_{AFM} = 74$ K and a weak ferromagnetic moment below 54 K. ESR measurements of the powder sample were carried out for several temperatures and frequencies to determine the g-factor and the magnetic exaction gap. Our goal is to identify the origin of the ferromagnetic contribution with ESR. We observe an opening of the ferromagnetic gap at T=93 K ($> T_{AFM}$) which continuously develops over the T_{AFM} down to low temperature. The complex interaction of the Cu- and Ir-spin gives rise to the continuous shift of the g-factor: By decreasing the temperature, the Ir spins are getting progressively more involved in the resonance of the statically ordered Cu spin lattice due to exchange coupling between the two sublattices. We conclude that the weak ferromagnetic component in La_2CuIrO_6 is intrinsic which points at a noncollinear spin-structure in the ordered state.

TT 78.19 Thu 15:00 Poster D

Investigation of the Thermodynamic Properties of Insulating Pyrochlores — •J. Gronemann[1,2], E. L. Green[1], R. Schönemann[1,2], M. Uhlarz[1], H.D. Zhou[3], M. Ruminy[4], T. Fennell[4], M. Kenzelmann[4], and J. Wosnitza[1,2] — [1]HLD-EMFL, HZDR, Dresden, Germany — [2]TU Dresden, Germany — [3]Univ. of Tennessee, Knoxville, USA — [4]PSI, Villingen, Switzerland

Geometrically frustrated pyrochlores have gained interest in recent years due to their novel low temperature properties. In the insulating compounds $Pr_2Sn_2O_7$ and $Tb_2Ti_2O_7$ the magnetic Pr^{3+} and Tb^{3+} ions form corner sharing tetrahedrons and can develop long or short-range order corresponding to a spin-ice or spin-liquid state, respectively. Heat capacity was measured down to 100 mK to investigate the low temperature ground state. Despite the similarities between both samples (similar crystal structures and a non-Kramers doublet in the ground state [1-2]) our measurements show no long-range magnetic order in $Tb_2Ti_2O_7$ down to 100 mK, a possible spin-liquid candidate, while in contrast $Pr_2Sn_2O_7$ is a well-known "dynamic" spin-ice compound as evidenced by a sharp specific heat anomaly around 800 mK [2] and confirmed by our recent AC susceptibility measurements. Though in typical spin-ice compounds the anomaly is suppressed by applying high magnetic fields, in $Pr_2Sn_2O_7$, however, the peak broadens and shifts to higher temperatures with increasing field. Further investigations are underway to determine the exact nature of this state and why it differs so drastically from the isostructural $Tb_2Ti_2O_7$.
[1] L. Ventelon et al., PRB **91**, 224430 (2015)
[2] H. D. Zhou et al., PRL **101**, 227204 (2008)

TT 78.20 Thu 15:00 Poster D

Spin-strain effects in the frustrated magnet $Tb_2Ti_2O_7$ at low temperatures — •Y. Gritsenko[1,2], S. Zherlitsyn[1], J. Wosnitza[1,2], M. Ruminy[3], T. Fennell[3], and M. Kenzelmann[4] — [1]HZDR/HLD, Dresden, Germany — [2]TUD/IFP, Dresden, Germany — [3]PSI/LNS, 5232 Villigen PSI, Switzerland — [4]PSI/LDM, 5232 Villigen PSI, Switzerland

Geometrically frustrated magnets have attracted much attention, due to their tendency to build unconventional ground states with exotic excitations. $Tb_2Ti_2O_7$ possesses a pyrochlore lattice as building block of the crystallographic structure, providing a basis for geometric frustration. This cubic material features Curie-Weiss temperature of $\Theta_{CW} = -19$ K, but no long-range magnetic order has been detected down to 50 mK indicating a large frustration. The existence of a spin-liquid state has been suggested for $Tb_2Ti_2O_7$. Here, we present results of ultrasonic investigations of this material. The magnetic field was applied along the [110] direction at temperatures of 20, 150 and 300 mK. Clear anomalies were found for different acoustic modes. The temperature dependence of the sound velocity shows a softening at about 500 mK and step-like features at about 150 mK suggesting a low-temperature phase transformation. This investigation sheds new light on the role of lattice degrees of freedom and magneto-elastic interactions in this material.

This work has been partially supported by DFG through SFB 1143. We acknowledge the support of the HLD at HZDR, member of the European Magnetic Field Laboratory (EMFL).

TT 78.21 Thu 15:00 Poster D

Magnetization of pyrochlore compounds at mK temperatures — •Lars Opherden[1,2], Thomas Herrmannsdörfer[1], Jianhui Xu[3], Nazmul Islam[3], Bella Lake[3], and Joachim Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden, HZDR, Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Abteilung Quantenphänomene in neuen Materialien, HZB, Berlin, Germany

Since spin-ice and magnetic-monopole behavior was observed in $Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$, frustrated $A_2B_2O_7$ (A = rare-earth, B = transition metal) pyrochlores became a highly topical research area [1]. In this material class, magnetic A^{3+} ions sit on corner-sharing tetrahedra. The crystal electrical fields dominate the interaction. This results in the formation of Kramer doublets and the alignment of the moments along the local ⟨111⟩ direction, if the rare-earth ions have a odd number of unpaired electrons. The balance between dipole-dipole and ferro- or antiferromagnetic exchange interaction leads to the occurrence of highly frustrated magnetism with a variety of ground state configurations such as spin-ice, spin-liquid or all-in-all-out ordering [2]. Because the correlation temperature is mostly observed at $T < 1$ K, magnetization measurements at millikelvin (mK) temperatures are necessary to investigate these ground states. Here, we present measurements performed in a SQUID magnetometer, designed for the mK temperature range, on novel pyrochlore zirconates $A_2Zr_2O_7$ (A = Nd, Sm).
[1] S. T. Bramwell *et. al.*, Science **294**, 1495 (2001).
[2] J. S. Gardner *et. al.*, Rev. Mod. Phys. **82**, 5546 (2010).

TT 78.22 Thu 15:00 Poster D

NMR of the frustrated spin-ladder system copper-sulfolane — •D. Dmytriieva[1], Z. Zhang[1], M. Naumann[1], H. Kühne[1], J. Wosnitza[1], E. Wulf[2], and A. Zheludev[2] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Neutron Scattering and Magnetism, Laboratory for Solid State Physics, ETH Zürich, Switzerland

We present first results from NMR experiments on the frustrated spin-ladder compound $H_8C_4SO_2{\cdot}Cu_2Cl_4$ (copper-sulfolane). From a comparison of the ^{35}Cl NMR spectra to macroscopic susceptibility data, we demonstrate that the ^{35}Cl nuclei are suitable local probes for the magnetic correlations of the nearby Cu^{2+} $S = 1/2$ moments. At magnetic fields exceeding 3.75 T and temperatures approaching 1.6 K, we find an

increase of the nuclear spin-lattice relaxation rate, signaling the onset of long-range magnetic order. For the structurally disordered version of this compound, specific-heat measurements indicate a strong suppression of the magnetic ordering temperature with surprisingly small concentrations of bromine substitution on the non-magnetic halogen site. It has been proposed that this phenomenology is driven by a novel mechanism, based on random frustration by bond disorder. In an approach to shed light on the substitution-induced modification of exchange couplings and correlations in the vicinity of the bromine sites as well as on the slow, long-range magnetic fluctuations at the transition to the ordered state, we show first results of ^{35}Cl and ^{81}Br NMR data obtained from high-quality single crystals.

TT 78.23 Thu 15:00 Poster D

Coexistence of spin frozen state and persistent spin dynamics in $NaSrCo_2F_7$ as probed by μSR and NMR — •Shanu Dengre[1], Rajib Sarkar[1], Sascha Albert Bräuninger[1], Jason W. Krizan[2], Felix Brückner[1], Philipp Materne[1], Hubertus Luetkens[3], Chris Baines[3], Hans-Henning Klauss[1], and Robert J. Cava[2] — [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

^{23}Na -and ^{19}F NMR, and μSR experiments are performed to explore the microscopic properties of $NaSrCo_2F_7$, which is a newly discovered magnetically frustrated pyrochlore with weak bond disorder and with a frustration index of f = 42. While ^{23}Na and ^{19}F NMR experiments clearly suggest the presence of quasi static field distribution below ∼3 K as reflected in the huge NMR line broadening and wipe out effect of NMR signal intensity, μSR experiments on the other hand remains passive to this spin frozen state. Both NMR and μSR results indicate the slowing down of the magnetic (spin) fluctuations upon cooling towards the NMR spin frozen state. μSR relaxation rate increases slightly below ∼ 3 K, and remains not only constant down to 20 mK, but also stands independent in longitudinal magnetic field upto 4000 G implying that the spin fluctuations are dynamic. These observations suggest the coexistence of partial spin frozen state and persistent spin dynamics in $NaSrCo_2F_7$.

TT 78.24 Thu 15:00 Poster D

Spin Dynamics in the Strongly Magnetically Frustrated Compounds $YBaCo_3AlO_7$ and $YBaCo_3FeO_7$ Probed by NMR and ESR Spectroscopy — •Margarita Iakovleva[1,2,4], Julian Zeisner[1,2], Martin Valldor[3], Evgeniia Vavilova[4], Hans-Joachim Grafe[1], Stephan Zimmermann[1,2], Alexey Alfonsov[1], Vladislav Kataev[1], and Bernd Büchner[1,2] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [4]E. K. Zavoisky Physical-Technical Institute, Kazan, Russia

In the Swedenborgite type compounds $YBaCo_3AlO_7$ and $YBaCo_3FeO_7$ the magnetic lattice can be described as a stacking of kagome layers, where unconventional ground states such as a spin liquid state can be expected due to the strong geometrical frustration. We performed a combined experimental study of magnetic properties of single crystals of $YBaCo_3AlO_7$ and $YBaCo_3FeO_7$ with high field ESR and high field NMR spectroscopy. The experimental results show the occurrence of short-range quasi static electron spin correlations at $T^* \approx 22$ K for $YBaCo_3AlO_7$ and $T^* \approx 60$K for $YBaCo_3FeO_7$ but not a long-range antiferromagnetic order. We compare our results with AC and DC susceptibility measurements and discuss a possible competition between a spin glass-like state due to intrinsic structural disorder and a spin liquid state arising from strong magnetic frustration in this materials.

TT 78.25 Thu 15:00 Poster D

Magnetic domains and frustration in metallic CePdAl — •Stefan Lucas[1], Zita Hüsges[1], Veronika Fritsch[2], Akito Sakai[2], Kai Grube[3], Christian Taubenheim[3], Chien-Lung Huang[1], Hilbert von Löhneysen[3], and Oliver Stockert[1] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]EP 6, Electronic Correlations and Magnetism, University of Augsburg, Germany — [3]Karlsruhe Institute of Technology, Germany

Magnetic frustration is an exciting topic in condensed matter physics, since it can lead to new ground states of materials, e.g. a spin liquid or spin glass state. Effects of magnetic frustration have been investigated intensively for insulating materials. However, the existence of magnetic frustration in metallic systems is still under debate. CePdAl is a metallic Kondo system, where geometric magnetic frustration arises from the formation of Ce ions on a distorted Kagomé lattice. Neutron scattering experiments revealed, that only two thirds of the magnetic Ce moments order antiferromagnetically below $T_N = 2.7$ K, whereas the other third remains mainly disordered. Thermodynamic as well as neutron scattering measurements are presented to verify the existence of partial magnetic frustration in CePdAl. Recently neutron diffraction experiments under magnetic fields applied along two orthogonal directions in the magnetically hard basal plane were performed. They show opposite effects on the magnetic intensity of a selected magnetic domain depending on the field direction with respect to the propagation vector. If this is only an effect of different domain population or also due to a change in magnetic frustration shall be discussed.

TT 78.26 Thu 15:00 Poster D

Numerical evidence for quadrupolar-octopolar order in $RETM_2(Al,Zi)_{20}$ — •Jan Attig[1], Darrell Tse[2], Eric Kin-Ho Lee[2], Arun Paramekanti[2], and Yong Baek Kim[2] — [1]Institute for Theoretical Physics, University of Cologne — [2]Department of Physics, University of Toronto, Toronto, Ontario M5S 1A7, Canada

Motivated by recent experiments on materials of the type $RETM_2(Al,Zi)_{20}$ (where RE is a rare earth and TM a transition metal element) we investigate a minimal model for the pseudo-spin degrees of freedom of the rare earth ions. The model is described by J1-J2 pseudo-spin interactions in three-dimensions where the XY part models quadrupolar order and the Ising part models octopolar order.

We use various computational methods such as simulating annealing to find the zero temperature phase digram and investigate further by using single-spin flip Monte Carlo simulations for finite temperature. One notable finding is the existence of non-coplanar spiral ordering of pseudo-spins, which may explain some of the experimental data on the electronic ordering in $RETM_2(Al,Zi)_{20}$.

TT 78.27 Thu 15:00 Poster D

Interplay of structural and magnetic properties in copper(II) sulfate hydrates $CuSO_4 \times nH_2O$ — Maria Rosner[1,2], Anne Henschel[1], Yurii Prots[1], Marcus Schmidt[1], •Helge Rosner[1], and Andreas Leithe-Jasper[1] — [1]MPI CPfS Dresden, Germany — [2]Martin-Andersen-Nexö-Gymnasium Dresden

Copper(II)-sulfate pentahydrate $CuSO_4 \times 5H_2O$ is likely the most abundant Cu(II) compound and well studied, including its quasi one-dimensional spin 1/2 magnetism. However, copper(II)-sulfates exist as a series of compounds $CuSO_4 \times nH_2O$ (n=0,1,3,5) that differ in their degree of hydration, exhibiting very distinct crystal structures and, in consequence, pronounced differences in their properties. Here, we present a systematic investigation of the series, comprising synthesis (powder and single crystals) , structural (XRD) and thermodynamical (DTA/TG, C_p, χ) characterization as well as electronic structure calculations. As the result, we obtain a consistent picture of the development of the magnetic behavior upon dehydration.

TT 78.28 Thu 15:00 Poster D

Fragmented S=1/2 alternating spin chains in layered monoclinic $Li_3Cu_2SbO_6$ — •Michael Richter[1], Changhyun Koo[1], Vladimir Nalbandyan[2], Elena Zvereva[3], Alexander Vasiliev[3], Igor Shukaev[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Chemistry Faculty, Southern Federal University, Rostov-na-Donu, Russia — [3]Faculty of Physics, Moscow State University, Moscow, Russia

We report the magnetic properties of polycrystalline layered $Li_3Cu_2SbO_6$ which reveals the coexistence of alternating $S = 1/2$ spin chains, spin chain fragments and quasi-free spins. Static magnetic susceptibility measurements show two contributions to the magnetic response, namely quasi-free spins at low-temperature and a spin-gapped magnetic subsystem with $\Delta \sim 120$ K. Quantitatively, the data imply that about half of the spins are organized in alternating Heisenberg chains with $J_1 = 75$ K and $J_2/J_1 = 0.6$. Our X-band ESR data corroborate well with this analysis by indicating three resolved resonance modes. High-frequency ESR shows powder-like spectra which are well described by an anisotropic g-factor with $g_\parallel = 2.31$ and $g_\perp = 2.05$. The magnetic response is ascribed to significant antisite disorder between Li and Cu-sites which yields quasi-free $S = 1/2$ spins at Li-sites as well as fragmentation of the spin chains in the Cu-layers.

TT 78.29 Thu 15:00 Poster D

Effect of explicit oxygen screening in the three-orbital

cuprate model — •Xiaodong Cao[1], Cornelia Hille[2], Priyanka Seth[3], Thomas Ayral[3,4], Olivier Parcollet[3], Sabine Andergassen[2], and Philipp Hansmann[1] — [1]Max-Planck-Institute for Solid State Research Heisenbergstr. 1, 70569 Stuttgart , Germany — [2]Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [3]Institut de Physique Théorique(IPhT), CEA, CNRS, 91191Gif-sur-Yvette, Franc — [4]Centre de Physique Théorique, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France

In the theoretical treatment of transition metal oxides we are always confronted with the question how important oxygen degrees of freedom are for ground state properties and low lying excitations. Different strategies have been employed in the past which can be separated into approaches that treat oxygen either implicitly as part of the effective transition metal 3d Wannier function or explicitly as non-interacting bath where correlated 3d states are "embedded". In the presented DMFT study we promote oxygen degrees of freedom to be active players for the correlated subspace by means of an RPA screening of the effective d-interaction which is now dynamic and included in a self-consistent way.

TT 78.30 Thu 15:00 Poster D

Electron Spin Resonance Spectroscopy on the Quasi-One-Dimensional Spin Chain Compound $Cu(NC_5H_5)_2(Cl_{1-x}Br_x)_2$ (x = 1.0, 0.98, 0.95) — •Julian Zeisner[1,2], Stephan Zimmermann[1,2], Vladislav Kataev[1], Michael Brockmann[3], Frank Göhmann[3], Michael Karbach[3], Andreas Klümper[3], Alexander Weisse[4], Matthias Thede[5], Andrey Zheludev[5], and Bernd Büchner[1,2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Bergische Universität Wuppertal, Wuppertal, Germany — [4]Max-Planck-Institut für Mathematik, Bonn, Germany — [5]ETH Zürich, Zürich, Switzerland

Although known for decades low dimensional magnetic systems remain an active field in modern solid state physics. Among other aspects this is due to the peculiarities arising in reduced dimensions which complicated correct theoretical descriptions of such systems. Recently, however, progress was made in exact calculation of electron spin resonance (ESR) properties based on a Heisenberg-Ising Hamiltonian [1]. In our work we present a comparison of these predictions with ESR studies on the quasi-one-dimensional magnet $Cu(NC_5H_5)_2Br_2$. Measurements were performed over a wide frequency and temperature range giving insight into spin dynamics as well as spin structure and the magnetic anisotropy present in this compound. In addition the impact of a partial substitution of Br by Cl on spin dynamics is shown.

[1] M. Brockmann, F. Göhmann, M. Karbach, A. Klümper, and A. Weiße, PRB **85**, 134438 (2012)

TT 78.31 Thu 15:00 Poster D

Optical investigations on spin liquids — •Mathias Bories — 1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

In quantum spin liquids, localized spins interact antiferromagnetically but without long-range order down to zero temperature due to quantum fluctuations. Anderson predicted this phase to have resonating valence bonds as ground state and spin 1/2 excitations called "spinons". However, experiments provided only recently evidence for its existence in a few materials, amongst which the triangular-lattice charge transfer salts κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ and EtMe$_3$Sb(Pd(dmit)$_2$)$_2$. Various measurements on these organic materials observed no long-range magnetic order down to the lowest temperatures which supports the proposed spin liquid behavior. Still, the nature of the ground state and its origin are still under debate. Theoretical studies have recently suggested a large spinon Fermi surface that could contribute to the optical conductivity by spin-charge interactions, leading to additional absorption within the Mott gap following a power-law frequency dependence.

We performed broadband spectroscopy at low temperatures covering the range from THz frequencies up to the visible. Special emphasis was put on the investigation of various compounds, including both inorganic and organic quantum spin liquid candidates, to possibly observe similarities or differences. The comparison gives us the possibility to pin down intrinsic features and thus enhance the current understanding of this phase, and possibly also trigger theoretical progress.

TT 78.32 Thu 15:00 Poster D

Optical investigations of disorder in spin liquids — •Miriam Sanz Alonso — 1.Physikalisches Institut, Stuttgart, Deutschland

Quantum spin liquids (QSL) emerge from frustrated spins on a triangular lattice with anitferromagnetic interaction. As proposed by Anderson, frustration prevents long range magnetic order down to lowest temperatures. In his model the ground state consists of resonating valence bonds (RVB) and is therefore highly degenerate. One of the most investigated QSL materials is the organic compound κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ which is a two-dimensional Mott insulator with triangular lattice. As it was also observed for closely related charge transfer salts, charge fluctuations may play a key role for the physical properties. Until now, this material was subject to magnetic, thermodynamic, transport and also some optical studies, supporting the proposed spin liquid behaviour. Recently, dielectric measurements observed typical fingerprints of relaxor ferroelectricity. Thus, we performed comprehensive spectroscopic investigations in the mid-infrared to track the temperature dependence of a charge-sensitive molecular vibration. As a result, sizeable charge disproportionation between the BEDT-TTF sites can be ruled out. In addition, we observed similar behavior in the closely-related compound κ-(BEDT-TTF)$_2$Ag$_2$(CN)$_3$. To examine the influence of disorder on the ground state, parameters like the cooling rate and chemical composition of the donor layer were varied.

TT 78.33 Thu 15:00 Poster D

Cluster Perturbation Theory for Spin Systems — •Benjamin Lenz, Salvatore R. Manmana, and Thomas Pruschke — Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany

Quantum cluster methods such as Cluster Perturbation Theory (CPT) or Variational Cluster Approximation (VCA) have been broadly applied to electron systems, but there are just very few applications to spin systems so far. Using Larkin's equations, a first order perturbation theory in cluster-cluster interactions can be constructed for spin systems and in a first attempt, dimerized Heisenberg chains have been addressed within CPT [1]. Here, we first benchmark the spectral functions and magnetization curves obtained for the Heisenberg XXZ chain by checking with exact Bethe ansatz results. Furthermore, we present CPT studies on Heisenberg zig-zag-ladders, which possess intriguing properties at high magnetic fields, and compare our findings with exact diagonalization.

Financial support via DFG through FOR1807 is gratefully acknowledged.

[1] A. S. Ovchinnikov, I. G. Bostrem, V. E. Sinitsyn, Theor. Math. Phys. **162**, 179 (2010).

TT 78.34 Thu 15:00 Poster D

Phase diagram of negative-hopping Bose-Hubbard model on triangular lattice — •Shijie Hu[1], Xuefeng Zhang[2], Axel Pelster[1], and Sebastian Eggert[1] — [1]Department of Physics and Research Center Optimas, Technical University Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Max Planck Institute for the Physics of Complex Systems Nöthnitzer Str. 38, 01187 Dresden, Germany

We study the phase diagram of the negative-hopping Bose-Hubbard model on the triangular lattice by using the parallel-tempering algorithm in the two-dimensional density matrix renormalization group (DMRG) method. For the integer-1 filling, we found a first-order transition from the chiral superfluid phase to the normal insulating phase where both U(1) and Z2 symmetry are spontaneously broken. Away from the integer-1 filling, we found a new phase corresponding to a kind of novel bond order. As the chemical potential increases, the negative-hopping Bose-Hubbard model undergoes two first-order transitions instead.

TT 78.35 Thu 15:00 Poster D

Variational Cluster Approximation for Iridates — •Teresa Schaller and Maria Daghofer — FMQ, Universität Stuttgart

We use the variational cluster approximation to investigate the phase diagram and one-particle spectral density of iridates, where kinetic energy, electronic interactions and spin-orbit coupling are all on comparable energy scales. The approach includes quantum fluctuations on a small cluster and exactly and included long-range order on a mean-field level. We will in particular investigate the filling of two holes in the t_{2g} subshell, as is realized in some iridium compounds. Hund's rule and spin-orbit coupling together favor then a local singlet ground state, while intersite exchange driven by the kinetic energy favors mag-

netism. We present the phase diagram resulting from this competition and the impact of crystal-field splitting.

TT 78.36 Thu 15:00 Poster D

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 based on a self-energy approach can be used to study correlated-electron Hamiltonians: The self-energy of the system is replaced by that of a 'reference system' that has to have the same interaction, but can have different kinetic energy. In practice, the reference system consists of isolated clusters, which restricts the class of accessible models to those, where the interaction is local, e.g., as in the Hubbard model. Inter-site interactions can be included exactly within each cluster, but not on bonds connecting clusters.

We propose here to use a mean-field decoupling for these bonds. While this is an approximation that falls ouside the self-energy approach, a systematic improvement over simple mean-field treatments becomes possible, as fewer bonds are mean-field decoupled for larger directly solved clusters. We present first results of this extension for the t-J-U model.

TT 78.37 Thu 15:00 Poster D

Magnetic Excitations of Spin-Orbit and Hund's Rule Coupled Mott Insulators — •Michael Schmid and Maria Daghofer — FMQ Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

When both, Hund's-rule and spin-orbit coupling are strong, the local ground state of two electrons in d^4 iridates is a singlet. However, the triplet states are not very high in energy and kinetic-energy-driven interactions between ions can mix some triplet character into the overall ground state. We are here interested in mangetic excitaions of such compounds and complement an analytic approach based on the similarity to dimers with a numerical investigation. We make here use of a recently extension of a dynamical density-matrix embedding scheme to exciations.

TT 78.38 Thu 15:00 Poster D

Thermal transport in the Heisenberg-Kitaev model — •Alexandros Metavitsiadis and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

We study the finite temperature thermal transport properties of the Kitaev-Heisenberg two-leg spin ladder, within the framework of linear response theory. For simultaneously non-vanishing Kitaev and Heisenberg exchange, we present results from numerical techniques, namely Exact Diagonalization and the Quantum Typicality, to explore the parameter space. In the absence of Heisenberg interactions, the model is exactly solvable, and we support our numerical findings with analytical results. In addition, the large number of conservation laws allows a detailed analysis of the transport properties in different Hilbert space subsectors, classified by different Z_2 gauge flux configurations. Finally we will focus on the breaking of integrability with the onset of a Heisenberg coupling on the ladder, starting from purely Kitaev exchange.

TT 78.39 Thu 15:00 Poster D

Frustration and Interaction in complex 2-dimensional Systems — •Malte Harland[1], Mikhail Katsnelson[2], and Alexander Lichtenstein[1] — [1]University of Hamburg — [2]Radboud University Nijmegen

We present a study of magnetic frustration in the Hubbard model. Frustration effects are a highly debated topic, since they are assumed to reveal new phases, e.g. spin liquids. To control the degree of frustration we interpolate the nearest-neighbour – next-nearest-neighbour hopping ratio of the square lattice. We choose a special 2d-lattice such, that the next-nearest-neighbour hopping exists only in every second square and is checkerboard-like distributed. We solve the half-filled Hubbard model and characterize different phases by means of the Cluster Dynamical Mean-Field Theory(CDMFT) for small, intermediate and large local Hubbard interactions. CDMFT maps the lattice problem onto a cluster in the Anderson-impurity model, that is solved numerically by a continuous-time quantum Monte Carlo solver (CTHYB). CDMFT enables us to investigate the non-local, short-range correlations of this frustrated system.

TT 78.40 Thu 15:00 Poster D

Dynamical mean-field and density-matrix renormalization-group studies of partial Kondo screening — •Matthias Peschke[1], Maximilian Aulbach[1], Fakher F. Assaad[2], and Michael Potthoff[1] — [1]I. Institut f. Theor. Physik, Universität Hamburg, Germany — [2]Institut f. Theor. Physik und Astrophysik, Universität Würzburg

The competition between Kondo screening and indirect magnetic exchange is studied for systems with geometrical frustration using dynamical mean-field theory (DMFT) and the density-matrix renormalization group (DMRG). A systematic scan of the weak- to intermediate-coupling regime of the periodic Anderson model on the triangular lattice is performed for a wide range of fillings n by means of a site-dependent DMFT approach for a non-primitive unit cell containing three correlated f orbitals. The resulting phase diagram comprises different phases: a non-magnetic Kondo insulator at half-filling, a non-magnetic metallic Kondo-singlet phase for fillings slightly off half-filling and an antiferromagnetic phase at lower fillings driven by RKKY exchange. The antiferromagnetic and the Kondo-singlet phases are separated in the U-n phase diagram by an extended region of partial Kondo screening (PKS), i.e., a phase where the magnetic moment at one site in the unit cell is Kondo screened while the remaining two are coupled antiferromagnetically. The mean-field scenario is checked against numerically exact DMRG data. To this end we analyze different two- and four-point magnetic correlation functions for the Kondo-lattice on one-dimensional frustrated ladders.

TT 78.41 Thu 15:00 Poster D

Phonons in the helimagnet MnSi — •Matthias Mörtter, Frank Weber, and Daniel Lamago — Karlsruher Institut für Technologie, Institut für Festkörperphysik, Deutschland

The interactions of electronic, spin, and lattice degrees of freedom in solids result in complex phase diagrams, new emergent phenomena, and technical applications. Recently, it was shown by detailed inelastic neutron scattering measurements and ab-initio calculations that the phonon renormalization in non-centrosymmetric FeSi is intimately linked to its unconventional magnetic properties [1]. In the current study, we investigated the isostructural helimagnet MnSi over a large temperature range, 4 K $\leq$ T $\leq$ 500 K, using thermal inelastic neutron scattering. Focusing on wave vectors with clear phonon selection rules, we report phonons energies, line widths and intensities and compare them to the magnetic properties of MnSi.

[1] S. Krannich et al., Nature Comm. **6**, 9961 (2015).

TT 78.42 Thu 15:00 Poster D

Andreev transport in a correlated ferromagnet-quantum-dot-superconductor device — •Krzysztof P. Wójcik and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland

In this contribution the spin-resolved Andreev transport in a hybrid ferromagnet-quantum-dot-superconductor device is discussed. In particular, the Andreev transmission and the resulting linear response conductance, calculated by means of the numerical renormalization group method, are analyzed. We show that, generally, the transport properties are conditioned by the interplay of correlations leading to the Kondo effect, superconducting proximity effect and the ferromagnetic-contact-induced exchange field. The exchange field greatly affects the low-energy behavior of the Andreev transmission by splitting the Kondo resonance. Moreover, it leads to a nonmonotonic dependence of the Andreev conductance on the dot level position. At low temperatures, the conductance has a peak at the particle-hole symmetry point, which however becomes quickly suppressed with increasing the temperature.

TT 78.43 Thu 15:00 Poster D

Magnetic Linear Dichroism of Collective Spin Excitations in a Chiral Magnet — •Ioannis Stasinopoulos[1], Stefan Weichselbaumer[1], Andreas Bauer[2], Helmuth Berger[3], Johannes Waizner[4], Markus Garst[4], Christian Pfleiderer[2] und Dirk Grundler[1,5] — [1]Physik-Department E10, TU München, Garching, Germany — [2]Physik-Department E51, TU München, Garching, Germany — [3]IMX, EPFL, Lausanne, Switzerland — [4]Institute for Theoretical Physics, Univ. Köln, Köln, Germany — [5]LMGN, IMX, EPFL, Lausanne, Switzerland

Skyrmions are spin whirls emerging in chiral-magnets and arranging in a hexagonal lattice with typical lattice constants of several tens of nm. Collective spin excitations in chiral magnets have generated large interest due to their potential for magnetologic and microwave appli-

cations. We describe the dynamics of the mean magnetization of the spin helix by considering the ellipticity and gyrotropy of its precession where we find magnetic linear dichroism over a remarkably large parameter range. Combining our calculations with broadband microwave spectroscopy on the insulator Cu_2OSeO_3, we demonstrate how to deliberately address different skyrmion or spin helix modes and induce finite wavevector transfer by using different coplanar waveguides and appropriate sample shapes. This detailed understanding allows to tailor the GHz response of chiral magnets for magnonic and spintronic devices.

Financial support by the DFG via TRR80 and NIM is acknowledged.

TT 78.44 Thu 15:00 Poster D

Correlations of magnetic crystalline order in critical chiral paramagnets — •Laura Köhler, Achim Rosch, and Markus Garst — Institute for theoretical physics, University of Cologne, Cologne, Germany

The formation of magnetic long-range order in chiral magnets like MnSi or Cu_3OSeO_3 corresponds to a so-called weak-crystallization process where strong interactions between critical paramagnons result in a fluctuation-induced first-order transition [1,2,3]. In these materials, the helimagnetic order and the Skyrmion lattice realize a one- and two-dimensional magnetic crystal, respectively. We explore crystalline correlations above the critical temperature T_c by considering the two-loop self-energy that involves three paramagnons with vanishing total momentum. In this case, the momenta of the paramagnons form a triangle. We discuss the importance of various triangular configuration and, in particular, equilateral triangles which are building blocks for two- as well as three-dimensional crystalline order.

[1] M. Janoschek et al., PRB **87**, 134407 (2013).
[2] A. Bauer, M. Garst and C. Pfleiderer, PRL **110**, 177207 (2013).
[3] J. Kindervater et al., PRB **89**, 180408(R) (2014).

TT 78.45 Thu 15:00 Poster D

Spin-wave excitations of magnetic skyrmion crystals — •Johannes Waizner and Markus Garst — Institute for Theoretical Physics, University of Cologne, Cologne, Germany

The cubic chiral magnets realize magnetic skyrmion crystals that correspond to topologically non-trivial, two-dimensional magnetic textures within the plane perpendicular to the applied field. The magnon excitations form, according to Bloch's theorem, a two-dimensional band structure. First, we focus on the magnetic resonances at the Gamma point [1] and discuss their properties, in particular, their ellipticity and gyrotropy. Second, we evaluate the energy- and momentum-dependent cross section expected in inelastic neutron scattering experiments. Third, we discuss the non-trivial topology of the magnon band structure that is reflected in finite Chern numbers of some of the bands.

[1] T. Schwarze, J. Waizner, M. Garst, A. Bauer, I. Stasinopoulos, H. Berger, C. Pfleiderer, and D. Grundler, Nat. Mater. **14**, 478 (2015).

TT 78.46 Thu 15:00 Poster D

Skyrmion caloritronics — •Sarah Schroeter, Achim Rosch, and Markus Garst — Institute for Theoretical Physics, Cologne, Germany

Skyrmions in insulating chiral magnets can be manipulated by applying a magnon current, for example, with the help of a temperature gradient. In turn, the scattering of spin-waves off skyrmions results in an emergent Lorentz force that leads to a topological magnon Hall effect. Based on our previous work [1,2], we discuss thermal transport of magnons in the presence of a dilute gas of skyrmions in a two-dimensional chiral magnet. Using the Boltzmann equation, we derive the thermal transport coefficients for the magnons as well as the effective equation of motion for the skyrmion positions.

[1] C. Schütte and M. Garst, PRB **90**, 094423 (2014).
[2] S. Schroeter and M. Garst, Low Temp. Phys. **41**, 817 (2015).

TT 78.47 Thu 15:00 Poster D

Spin chains with weak dissipation and pumping — •Florian Lange, Zala Lenarčič, and Achim Rosch — Universität zu Köln

We consider one-dimensional spin chains weakly coupled to the environment. The coupling is described by a Lindblad equation. Such a setup could, for example, be spin chains coupled to a bath of nuclear spins, by ultracold atoms or by atoms in cavities. In the limit of weak coupling, the steady state density matrix is approximately described by a (generalized) Gibbs ensemble. The parameters of this ensemble are obtained by tracking the evolution of the (approximate) conservation laws of the system arising from the coupling to the bath. Details of the couplings strongly influence the steady state and the system can be tuned to low, high or negative temperatures. Integrable and non-integrable spin chains show qualitatively different behaviour.

TT 78.48 Thu 15:00 Poster D

The Fermi surface of Sr_2RuO_4: spin-orbit and anisotropic Coulomb interaction effects — Guoren Zhang, Evgeny Gorelov, •Esmaeel Sarvestani, and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Juelich, D-52425 Juelich, Germany

The topology of the Fermi surface of Sr_2RuO_4 is well described by local density approximation calculations with spin-orbit interaction, but the relative size of its different sheets is not. By accounting for many-body effects via dynamical mean-field theory, we show that the standard isotropic Coulomb interaction worsen or does not correct this discrepancy. In order to reproduce experiments, it is essential to include the Coulomb anisotropy. The latter is small but has strong effects; it competes with the Coulomb-enhanced spin-orbit coupling and with the isotropic Coulomb term. This mechanism is likely to be at work in other multi-orbital systems. Finally, we find a strong spin-orbital entanglement. This supports the view that the conventional description of Cooper pairs via factorized spin and orbital part might not apply to Sr_2RuO_4.

TT 78.49 Thu 15:00 Poster D

Highly Anisotropic Magnon Dispersion in Ca_2RuO_4: Evidence for Strong Spin Orbit Coupling — •Stefan Kunkemöller[1], Daniel Khomskii[1], Paul Steffens[2], Andrea Piovano[2], Augustinus Agung Nugroho[3], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut Laue Langevin, Grenoble, France — [3]Institut Teknologi Bandung, Indonesia

Ca_2RuO_4 is a key material for the understanding of the impact of spin-orbit coupling in 4d and 5d compounds, which is intensively studied at present. We have studied the magnon dispersion in Ca_2RuO_4 by inelastic neutron scattering on large single crystals containing 1

TT 78.50 Thu 15:00 Poster D

Temperature and polarization dependent Raman measurements of Ca_2RuO_4 — •Raphael German — II.Physikalisches Institut Köln

Ca_2RuO_4 is a Mott-like insulator, which undergoes a metal-insulator transition at 357 K and antiferromagnetic ordering at $T_N = 110$ K. Here, we report a temperature and polarization dependent Raman scattering study. Earlier studies claimed a Raman active two-magnon excitation around 100 cm^{-1}. This, however, is incompatible with the results from recent inelastic neutron scattering measurements, which suggest that this mode might be of single magnon nature. Instead, it is more likely that the feature which appears at ~ 650 cm^{-1}, previously claimed to be due to a charge gap, has a two-magnon origin. Another open question in the interpretation of the Raman spectra is the origin of the high-energy peak at ~ 1360 cm^{-1}. We will discuss the origin of the Raman peaks in terms of one- and two-magnon processes; magnon-phonon coupling, and possible crystal field excitations.

TT 78.51 Thu 15:00 Poster D

Field-induced ordered phases in the tetragonal quasi-2d dimer system $Ba_{0.9}Sr_{0.1}CuSi_2O_6$ — •Lars Postulka, Bernd Wolf, Pascal Puphal, Natalija Van Well, Franz Ritter, Cornelius Krellner, and Michael Lang — Goethe-Univeristät, Physikalisches Institut SFB/TR49, D-60438 Frankfurt(M),Germany

Magnetic compounds built of antiferromagnetically-coupled S = 1/2 dimers, allow to study finite-temperature critical phenomena under well-controlled conditions, including Luttinger-liquid, Berezinskii-Kosterlitz-Thouless-type topological order as well as Bose-Einstein-condensation of triplons. A material of high interest within this context is the quasi-2d coupled-dimer system $BaCuSi_2O_6$, which shows a field-induced ordered state exhibiting the signatures of a dimensional reduction [1]. This has been assigned to perfectly frustrated interlayer couplings, but has been questioned by Sheptyakov et al. since the system undergoes a tetragonal to orthorhombic phase transition at 100 K below which two different types of dimer layers exist [2]. Here we report magnetic properties of $Ba_{0.9}Sr_{0.1}CuSi_2O_6$ where the structural phase

transition has been suppressed by strontium doping. We show results on magnetic susceptibility measurements as a function of temperature between 2 K < T < 300 K as well as field-dependant measurements up to B < 50 T at T = 1.5 K. We estimate the magnetic couplings and compare the results with those of the well-known parent compound $BaCuSi_2O_6$.
[1] S. E. Sebastian et al., Nature **441**, 617 (2006)
[2] D. V. Sheptyakov et al., PRB **86**, 014433 (2012)

TT 78.52 Thu 15:00 Poster D

Dimensional crossover in manganese based analogues of iron pnictides — •Manuel Zingl, Elias Assmann, and Markus Aichhorn — Institute of Theoretical Physics and Computational Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

The manganese pnicitides $BaMn_2As_2$ and LaOMnAs crystallize in the same structure as the extensively studied iron pnictide high-temperature superconductors $BaFe_2As_2$ and LaOFeAs. In contrast to the d^6 configuration of the iron systems, the manganese d-shell is only half-filled (d^5). As a consequence, electronic correlations are much stronger, placing these compounds at the verge of the Mott metal-insulator transition. In this region of the phase diagram materials are prone to enhanced magnetism, apparent in the remarkably high Néel temperature of 625 K for $BaMn_2As_2$. We demonstrate that the experimentally observed differences in the Néel temperatures, the band gap, and the optical properties of the manganese compounds under consideration can be traced back to their effective dimensionality. Our fully charge self-consistent DFT+DMFT calculations show excellent agreement with experiments, especially measured optical spectra.

TT 78.53 Thu 15:00 Poster D

Electronic structure of Mo and W investigated with positron annihilation — •Markus Dutschke[1], Michael Sekania[1,3], Diana Benea[4,5], Hubert Ceeh[6], Joseph-A. Weber[6], Christoph Hugenschmidt[6], and Liviu Chioncel[1,2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [3]Andronikashvili Institute of Physics, Tamarashvili 6, 0177 Tbilisi, Georgia — [4]Faculty of Physics, Babes-Bolyai University, Kogalniceanustr 1, Ro-400084 Cluj-Napoca, Romania — [5]Department of Chemistry, Ludwig Maximilian University of Munich, Butenandstr. 5-13, D-81377 München, Germany — [6]FRM II, Technische Universität München, Lichtenbergstrasse 1 D-85748 Garching, Germany

We perform electronic structure calculations to analyze the momentum distribution of the transition metals molybdenum and tungsten. We study the influence of positron-electron and the electron-electron interactions on the shape of the two-dimensional angular correlation of positron annihilation radiation (2D-ACAR) spectra. Our analysis is performed within the framework of the combined Density Functional (DFT) and Dynamical Mean-Field Theory (DMFT). Computed spectra are compared with recent experimental investigations.

TT 78.54 Thu 15:00 Poster D

Infrared study of the electronic phase diagram of $Cr_{1-x}V_xN$ — Fabian Meggle[1], •Jihaan Ebad-Allah[1,2], Francisco Rivadulla[3,4], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Department of Physics, University of Tanta, 31527 Tanta, Egypt — [3]Center for Research in Biological Chemistry and Molecular Materials, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain — [4]Department of Physical Chemistry, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain

Transition-metal nitrides have attracted great interest due to their mechanical and physical properties, which are useful for improving technological applications [1]. Several studies suggested that doping CrN with vanadium could lead to thermoelectric materials, which have optimal mechanical and chemical properties. CrN is a narrow gap, correlation-induced, semiconductor. Increasing vanadium doping in $Cr_{1-x}V_xN$ leads to a gradual suppression of the resistivity and a transition to itinerant-electron behavior through several phases including superconductivity in VN [2].

Here we report the results of a study on the electronic and vibrational properties of $Cr_{1-x}V_xN$ powder pellets by reflection measurements in the infrared and visible frequency ranges at ambient conditions. Furthermore, we carried out resistivity measurements to confirm the behaviour of the optical conductivity at low energy.
[1] P. F. McMillan, Nature Materials **1**, 19 (2002)
[2] C. X. Quintela, F. Rivadulla, and J. Rivas, PRB **82**, 245201 (2010).

TT 78.55 Thu 15:00 Poster D

Crystal growth and characterization of Ir-Te compounds — •Philipp Kurzhals, Frank Weber, Diego Zocco, Peter Adelmann, Michael Merz, Thomas Wolf, Sebastian Kuntz, and Kai Grube — Karlsruhe Institute of Technology, Institute for Solid State Physics, Karlsruhe, Germany

$IrTe_2$ is distinguished by a structural phase transition whose origin is not understood up to the present day [1]. We grew crystals using the self-flux method starting from the reagents iriudium and tellurium and got specimen with varying amounts of $IrTe_2$ and Ir_3Te_8, analyzed by x-ray powder diffraction. We studied the transition near T = 280 K in magnetization measurements down to T = 1.8 K probing also for superconductivity, which was reported for intercalated samples [2]. Results indicate that the structural transition happens over an extended range in temperature and superconductivity is absent in our samples.

Ir_3Te_8 is not studied to such an extent as $IrTe_2$. In previous publications a structural phase transition is reported [3]. We characterized the transition by performing magnetization measurements and X-ray diffraction.
[1] G. L. Pascut et al., PRL **112**, 086402 (2014)
[2] J. J. Yang et al., PRL **108**, 116402 (2012)
[3] L. Li et al., PRB **87** (2013).

TT 78.56 Thu 15:00 Poster D

Angle-Resolved Photoemission Spectroscopy of rare earth $LaSb_2$ — Matteo Michiardi[1], •Fabian Arnold[1], G. Shwetha[2], V. Kanchana[2], Vaitheeswaran Ganapathy[3], Karl Frederik Faerch Fisher[1], Axel Svane[1], Marco Bianchi[1], Bo Brummerstedt Iversen[1], and Philip Hofmann[1] — [1]Aarhus University, Denmark — [2]IIT-Hyderabad, India — [3]University of Hyderabad, India

Several rare earth diantimonides have been found to exhibit intriguing electronic properties such as anisotropic linear and non-saturating magnetoresistance. Among these materials, $LaSb_2$ is not only considered for application in magnetoresistive devices but it is also found to be superconducting at low temperatures and it is investigated as candidate material to host charge density wave phases. Despite the several studies on its transport properties, the electronic structure of $LaSb_2$ is still largely unknown. Here we present an angle-resolved photoemission spectroscopy and ab-initio calculation study of $LaSb_2(001)$. The observed band structure is found to be in good agreement with theoretical predictions. Our results reveal that $LaSb_2$ is a semimetal with a strongly nested two-dimensional Fermi surface. The low energy spectrum is characterized by four massive hole pockets and by four shallow, strongly directional, electron pockets that exhibit Dirac-like dispersion. We speculate on the possibility that this peculiar electronic structure drives the magnetoresistance to its quantum limit, explaining its unconventional behavior.

TT 78.57 Thu 15:00 Poster D

Ground state properties of MnB_4 — •Jan Lennart Winter[1], Nico Steinki[1], Dirk Schulze Grachtrup[1], Dirk Menzel[1], Stefan Süllow[1], Arno Knappschneider[2], and Barbara Albert[2] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, TU Darmstadt, Germany

Recently, single crystalline MnB_4 was synthesized for the first time, yielding microscale crystals with dimensions of the order of 200 μm [1]. Based on band structure calculations, it was argued that the material is semiconducting as result of a Peierls distortion. Conversely, in a study of polycrystalline material it was concluded that the material is a weakly ferromagnetic metal [2].

To establish if MnB_4 is a semiconductor we have carried out single crystal four point resistivity measurements. For this purpose a setup for measuring microscale samples was developed and characterized. Qualitatively, we find semiconducting behavior (increasing resistivity for decreasing temperature), although a band gap could not be derived because of a non-linear Arrhenius plot. Our data are consistent with MnB_4 being a pseudogap/small gap material as proposed in [1]. A pronounced sample dependence of the transport properties points to the presence of impurity states. For the single crystals no ferromagnetic signatures could be obtained, suggesting an extrinsic cause of it in polycrystalline material.
[1] A. Knappschneider et al., Angew. Chem. **126**, 1710 (2014)

[2] H. Gou et al., PRB **89**, 064108 (2014)

TT 78.58 Thu 15:00 Poster D

Scaling of the Optical Conductivity in the Transition from Thermal to Many-Body Localized Phases — •Robin Steinigeweg[1], Jacek Herbrych[2], Frank Pollmann[3], and Wolfram Brenig[4] — [1]University of Osnabrück — [2]CCQCN and University of Crete — [3]MPIPKS Dresden — [4]Technical University Braunschweig

We study the frequency dependence of the optical conductivity $\mathrm{Re}\,\sigma(\omega)$ of the Heisenberg spin-1/2 chain in the transition from thermal to many-body localized phases induced by the strength of a spatially random magnetic field. Using the method of dynamical quantum typicality, we calculate the real-time dynamics of the spin-current autocorrelation function and obtain the Fourier transform $\mathrm{Re}\,\sigma(\omega)$ in high frequency resolution and for system sizes L much larger than $L \sim 14$ accessible to standard exact-diagonalization approaches. We unveil that the low-frequency behavior of $\mathrm{Re}\,\sigma(\omega)$ is well described by $\mathrm{Re}\,\sigma(\omega) \approx \sigma_{\mathrm{dc}} + a\,|\omega|^{\alpha}$, with $\alpha \approx 1$ in a wide range of the thermal phase and up to the many-body localized phase. We particularly detail the decrease of σ_{dc} as a function of increasing disorder for strong exchange anisotropies. We further find that the temperature dependence of σ_{dc} is consistent with the existence of a mobility edge.

TT 78.59 Thu 15:00 Poster D

Non-Equilibrium transport study in strongly correlated hetero structures — •Milos Radonjic[1,2], Ivan Rungger[3], and Liviu Chioncel[1] — [1]Center for Electronic Correlations and Magnetism, TP III, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — [3]Mathematics and Modelling, National Physical Laboratory, Hampton Rd, Teddington, Middlesex, UK, TW11 0LW

The effects of local electronic interactions and finite temperatures upon the non-equilibrium transport properties across the metallic heterostructure Cu_4CoCu_4 are studied. Results are obtained by combining DFT and equilibrium DMFT solver on one side, and DFT and non-equilibrium steady state impurity solver based on second order perturbation in Hubbard interaction U, on the other side. Results of these two methods are compared for the transmission. It is shown that local, but dynamical electronic correlations reduce the total transmission at the Fermi level, and also increase the spin polarization. The multi-orbital non-equilibrium steady state impurity solver is formulated in the Keldysh Green's function formalism and allows us an access to all non-equilibrium quantities, such as non-equilibrium steady state current.

TT 78.60 Thu 15:00 Poster D

Self-consistent Born approach to strongly correlated electron systems in non-equilibrium — •Gerhard Dorn — TU Graz, Austria

The self-consistent Born master equation method is apt to describe the non-equilibrium behaviour of strongly correlated electron systems which are weakly coupled to non-interacting leads.

The poster compares the self-consistent Born approach with different other methods, like Born Markov master equation or Cluster Perturbation Theory (CPT), and shows the improvements according to correct representation of the Coulomb blockade or of the lead induced level broadening.

TT 78.61 Thu 15:00 Poster D

Boundary-driven dissipative quantum chains in large external fields — •Zala Lenarcic[1] and Tomaz Prosen[2] — [1]Institute for theoretical physics, University of Cologne, D-50937, Germany — [2]Faculty for mathematics and physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia

We treat the nonequilibrium transport as a consequence of a combined driving: from a pseudo-force, originating in the bias in Markovian processes at the system's boundaries, and from a real force due to an external field gradient g. For strong field gradients a systematic perturbation theory of the steady state current and slowest decay modes of the density matrix can be formulated for a general inhomogeneous XXZ spin 1/2 chain. From the explicit asymptotic expression for the current it is clear that by combining both drivings arbitrarily large current rectification can be achieved under $g \to -g$ in the presence of interaction. Moreover, via tailored field profiles one can obtain further control over the strength of stationary current.

[1] Z. Lenarčič and T. Prosen, PRE **91**, 030103(R) (2015).

TT 78.62 Thu 15:00 Poster D

Combining ab initio wavefunction methods with dynamical mean-field theory: A feasibility study with NiO — •Daniil Toloui-Mantadakis, Marc Hoeppner, Theodoros Tsatsoulis, Andreas Grueneis, and Philipp Hansmann — Max Planck Institute for Solid State Research, Stuttgart, Germany

In materials science, Density Functional Theory has been proved to be, so far, the most reliable and efficient tool for computational simulations of compounds. Effects of electronic correlations, however, conflict with the effective single particle picture of DFT. The first step beyond - by means of perturbation theory - emerges in various implementations of the so called GW method, but also here computations are questionable in non-perturbative regimes, e.g., close to the Mott-Hubbard metal to insulator transition. Only computationally costly non-perturbative methods like dynamical mean-field theory can help to provide answers on reduced Hilbert spaces of effective Hamiltonians. The widely used combination of DMFT with DFT methods is, however, always confronted with the conceptual difference between the two approaches and the so called double counting errors cannot be avoided. In our study we replace DFT with Hartree-Fock or Hartree-Fock+MP2 theory which does not pose this problem when connected with DMFT. Retaining non-local self energies on a static mean field level we perform a feasibility study of fully self consistent HF+MP2+DMFT for the example of NiO.

TT 78.63 Thu 15:00 Poster D

Spin-Orbit functional renormalization for unconventional Fermi surface instabilities — •Mario Fink — Institut für Theoretische Physik und Astrophysik Lehrstuhl für Theoretische Physik I Am Hubland 97074 Würzburg

The functional renormalization group has been successfully employed to describe the pairing mechanism in e.g. the cuprates and iron pnictides. For the latter, the expansion to multi-orbital models proved both necessary and revealing, providing a concise microscopic understanding of the extended s-wave order parameter. As another aspect of complexity of the electronic band structure, spin-orbit coupling (SOC) has been identified as an essential ingredient for the appearance of topological superconductors and further intricate unconventional Fermi surface instabilities. We present an expanded scheme of the functional renormalization group that incorporates the coupling between orbital and spin degrees of freedom. We consider atomic SOC as well as Rashba SOC in order to explore unconventional phases that mix singlet and triplet pairing instabilities in the particle-particle and the particle-hole channel. We illustrate our approach at the example of representative multi-orbital spin-orbit models.

TT 79: Superconductivity: Fe-based Superconductors - 122

Time: Thursday 15:30–18:30 Location: H21

TT 79.1 Thu 15:30 H21

Magnetic Excitations in Na-doped $BaFe_2As_2$ — •Florian Wasser[1], Sabine Wurmehl[2], Saicharan Aswarthem[2], Yvan Sidis[3], Astrid Schneidewind[4,5], Jitae Park[5], Bernd Büchner[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zuKöln, Zülpicher Strasse 77, D-50937 Köln, Germany — [2]Institute for Solid State Research, IFW Dresden,D-01171 Dresden, Germany — [3]Laboratoire LéonBrillouin, CEA-CNRS, CEA Saclay, 91191 Gif-sr-Yvette Cedex,France — [4]Jülich Centre for Neutron Science-JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ,D-85747, Garching, Germany — [5]Forschungsneutronenquelle Heinz Maier-Leibnitz(FRM-II), TU München, D-85747 Garching, Germany

Our neutron scattering study of magnetic excitations in $Ba_{1-x}Na_xFe_2As_2$ show that the presence of static antiferromagnetic

(AFM) order dominates the low-energy part of the spectrum even in the superconducting (SC) state. In the coexistence regime i.e. at 35% and 39% Na-doping an additional sharp and intense low-energy resonance mode, centred at ∼4meV, develops below T_c. This low-energy resonance excitation is predominantly polarized along the *c*-direction, which corresponds to a longitudinal alignment due to the spin-reorientation in this material. In the SC phase the elastic AFM signal becomes strongly reduced suggesting that the corresponding spectral weight is shifted to higher energies and in particular to the development of the 4meV-mode. In contrast, at 40% Na-doping static AFM order is absent and the 4meV-mode is fully suppressed.

TT 79.2 Thu 15:45 H21

A light scattering study of detwinned $BaFe_2As_2$ — •Andreas Baum[1,2], Milan Tomić[3], Daniel Jost[1,2], Ali Özkü[1,2], Bernhard Muschler[1], Florian Kretzschmar[1,2], Thomas Böhm[1,2], Nitin Chelwani[1,2], Jiun-Haw Chu[4,5], Ian R. Fisher[4,5], Roser Valentí[3], and Rudi Hackl[1] — [1]Walther-Meissner-Institut, 85748 Garching, Germany — [2]Fakultät für Physik E23, Technische Universität München, 85748 Garching, Germany — [3]Institut für Theoretische Physik, Goethe-Universität Frankfurt — [4]SIMES, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — [5]GLAM and Department of Applied Physics, Stanford, University, Stanford, CA 94305, USA

The magneto-structural phase transition of $BaFe_2As_2$ is studied by Raman spectroscopy with a focus on lattice dynamics. Using uniaxial pressure to detwin the sample allows us to resolve anisotropic features. The As A_{1g} phonon shows a resonance at high energies with distinct differences between the antiferromagnetically and the ferromagnetically ordered direction. The splitting of the E_g phonon at 130 cm^{-1} into two modes having B_{2g} and B_{3g} symmetry can be attributed to the transition into the magnetically ordered state rather than the structural transition. Both effects can be attributed to the emergence of magnetic order by DFT calculations.

TT 79.3 Thu 16:00 H21

Electronic correlations in the hole-doped superconductor $RbFe_2As_2$ probed via ^{75}As NMR — •S. Molatta[1,2,3], Z. Zhang[1], D. Dmytriieva[1], S. Khim[4], S. Wurmehl[2,3,4], H.-J. Grafe[4], B. Büchner[2,3,4], H. Kühne[1], and J. Wosnitza[1,2,3] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]TU Dresden, Germany — [3]DFG GRK-1621 — [4]IFW Dresden, Germany

We will present latest ^{75}As NMR data in the normal state of the stoichiometric superconductor $RbFe_2As_2$. This will be put into context to known results for the heavily hole-doped compound KFe_2As_2. The static and dynamic magnetic correlations were probed via measurements of the Knight shift and nuclear spin-lattice relaxation rate in a wide temperature range from 0.3 to 300 K. Although neither a magnetic nor a structural transition were observed down to lowest temperatures, the very close proximity of the ground state to a magnetic instability is indicated by a pronounced Curie-Weiss-like behavior of spin fluctuations. At around 100 K, we find a maximum of the Knight shift and a changing exponent of the temperature-dependent relaxation rate. This is phenomenologically similar to the case of KFe_2As_2 and was proposed to stem from a incoherence-coherence crossover mechanism of electronic correlations.

TT 79.4 Thu 16:15 H21

Coexistence of superconductivity and magnetism in $Ca_{1-x}Na_xFe_2As_2$: Universal suppression of the magnetic order parameter in 122 iron pnictides — •Philipp Materne[1], Sirko Kamusella[1], Rajib Sarkar[1], Luminita Harnagea[2], Sabine Wurmehl[1,2], Bernd Büchner[1,2], Hubertus Luetkens[3], Carsten Timm[4], and Hans-Henning Klauss[1] — [1]IFP, TU Dresden, 01062 Dresden, Germany — [2]IFW Dresden, Postfach 270016, 01171 Dresden, Germany — [3]PSI, 5232 Villigen, Switzerland — [4]ITP, TU Dresden, 01062 Dresden, Germany

We examined $Ca_{1-x}Na_xFe_2As_2$ single crystals with $x = 0.00$, 0.35, 0.50, and 0.67 by means of muon spin relaxation and Mössbauer spectroscopy to investigate the electronic and structural properties of these compounds. $CaFe_2As_2$ is a semimetal, which shows spin density wave order below 167 K. By hole doping via Ca→Na substitution, the magnetic order is suppressed and superconductivity emerges with $T_c \approx 34$ K at optimal doping including a substitution level region where both phases coexist. We have studied the interplay of order parameters in this coexistence region and found nanoscopic coexistence of both order parameters. This is proven by a reduction of the magnetic order parameter by 7 % below the superconducting transition temperature. We present a systematic correlation between the reduction of the magnetic order parameter and the ratio of the transition temperatures, T_c/T_N, for the 122 family of the iron-based superconductors [1].

[1] Ph. Materne *et al.*, PRB **92**, 134511 (2015)

TT 79.5 Thu 16:30 H21

Reversible tuning of the collapsed tetragonal phase transition in $CaFe_2As_2$ by separate control of chemical pressure and electron doping — •kan zhao and philipp gegenwart — Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany

Single crystals of $Ca(Fe_{1-x}Ru_x)_2As_2$ ($0 \leq x \leq 0.065$) and $Ca_{1-y}La_y(Fe_{0.973}Ru_{0.027})_2As_2$ ($0 \leq y \leq 0.2$) have been synthesized and studied with respect to their structural, electronic and magnetic properties. The partial substitution of Fe by Ru induces a decrease of the c-axis constant leading for $x \sim 0.023$ to the suppression of the coupled magnetic and structural (tetragonal to orthorhombic) transitions. At $x_{cr} = 0.023$ a first order transition to a collapsed tetragonal (CT) phase is found, which behaves like a Fermi liquid and which is stabilized by further increase of x. The absence of superconductivity near xcr is consistent with truly hydrostatic pressure experiments on undoped $CaFe_2As_2$. Starting in the CT regime at x=0.027 we investigate the additional effect of electron doping by partial replacement of Ca by La. Most remarkably, with increasing y the CT phase transition is destabilized and the system is tuned back into a tetragonal ground state at $y \sim 0.08$. This effect is ascribed to a weakening of interlayer As-As bonds by electron doping. Upon further electron doping filamentary superconductivity with T_c of 41 K at y=0.2 is observed.

TT 79.6 Thu 16:45 H21

Charge dynamics of $BaFe_2(As_{1-x}P_x)_2$: infrared spectroscopy study under pressure — •Ece Uykur[1], Tatsuya Kobayashi[2], Wataru Hirata[2], Shigeki Miyasaka[2], Setsuko Tajima[2], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, D-86195 Augsburg, Germany — [2]Department of Physics, Graduate School of Science, Osaka University, Osaka 560-0043, Japan

Temperature-dependent reflectivity measurements under pressure (up to 5 GPa) have been performed on $BaFe_2(As_{1-x}P_x)_2$ single crystals with $x = 0$ and 0.20 between ∼ 85 - 7000 cm^{-1} down to 6 K. Normal state charge dynamics as well as the low temperature dynamics (magnetically ordered (SDW) state and superconducting (SC) state) under pressure have been investigated. At temperatures above the magnetic phase transition, the metallicity of the system is increasing with pressure. At lower temperatures, with increasing pressure the partial suppression of the SDW state and the appearance of the SC state (at around 3.6 GPa) is observed for the parent compound with $x = 0$. The coexisting of these two states has been clearly demonstrated. The results of this study indicate a possible competing order scenario for these two orders. On the other hand, for the compound with $x = 0.20$, the SDW state has been completely suppressed above 2.5 GPa. The normal state and the superconducting state in this compound will be discussed in comparison to the parent compound.

15 min. break

TT 79.7 Thu 17:15 H21

Shifted Van Hove singularities (VHS) vs. vicinity to a selective Mott transition in $K(Rb,Cs)Fe_2As_2$: How strong is the el.-el. interaction? — •Stefan-Ludwig Drechsler[1], Sergey Borisenko[1], Sabine Wurmehl[1], Seunghyun Khim[1], Bernd Buechner[1], Steffen Backes[2], Harald Jeschke[2], Roser Valenti[3], and Helge Rosner[3] — [1]ITF at the Leibniz Institute IFW-Dresden, 01171 Dresden, Germany — [2]Inst. f. Theor. Phys., University of Frankfurt, Germany — [3]MPI-CPfS, Dreden, Germany

We report high precision scalar and full relativistic DFT calculations for the title compounds to get a trustable starting point for the discussion of many-body effects which become visible in the mass enhancement and shifted position of various VHS as observed by ARPES and STM [1]. For KFe_2As_2 we observe a Fe $3d_{xz}$-$3d_{yz}$ VHS shift from ∼ 65 meV below the Fermi energy ε_F in the DFT to ∼ -14 meV in our ARPES data and a squezing by a factor of 2 pointing to a moderate mass enhancement for this subgroup of electrons. For the $3d_{xy}$ derived band a shift from -300 meV to -50 meV has been detected. The

shifted VHS contributes to an enlarged DOS at ε_F explaning in part the large Sommerfeld coefficient γ seen in el. specific heat data. In recent DMFT calculations [2] the VHS related DOS-maxima are even closer to ε_F for an Hubbard interaction $U_d = 4$ eV and Hund's rule coupling. We suggest that the systems under consideration are less strongly correlated as compared to sophisticated selective Mott and Kondo-like scenarios.

[1] D. Fang, *et al.*, PRB **92**, 144513 (2015)
[2] S. Backes, H. Jeschke, and R. Valenti, PRB **92**, 195128 (2015)

TT 79.8 Thu 17:30 H21

Charge doping versus impurity scattering in substitutionally disordered Ba-122 — •Alexander Herbig[1], Rolf Heid[1], and Jörg Schmalian[2,1] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie — [2]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie

The iron-based superconductors are a prominent example how chemical substitution can be used as a tuning parameter for the electronic properties and the superconductivity of a complex material. Until now, first principle calculations addressing disorder effects on the electronic structure via methods beyond supercells are rare. Also the role of doping and the impact of chemical substitution on superconductivity is not fully understood. Based on ealier work [1], we recently implemented Blackman, Esterling and Berk's [2] extension of the coherent potential approximation within a pseudopotential framework using a linear combination of atomic orbitals basis. We present electronic structure calculations for the Ba-122 compound using this method with various species substitutions at different sites and arbitrary impurity concentrations. We focus on disorder effects on electron and hole bands near the Fermi level. We observe non-rigid level shifts and band selective broadenings due to impurity scattering which strongly depend on the substituent species [3]. Our finding of an enhanced intraband compared to interband scattering is in accordance with an s^{+-} paring state.

[1] K. Koepernik et al., PRB **55**, 5729 (1997)
[2] J. A. Blackman et al., PRB **4**, 2412 (1971)
[3] A. Herbig et al., arXiv:1510.06941v1 (2015)

TT 79.9 Thu 17:45 H21

Angle-resolved photoemission spectroscopy calculations on antiferromagnetic $BaFe_2As_2$ and $Ba(Fe_{1-x}Co_x)_2As_2$ based on the one-step model — •Gerald Derondeau[1], Jürgen Braun[1], Ján Minár[1,2], and Hubert Ebert[1] — [1]Department Chemie, Ludwig-Maximilians-Universität München, 81377 München, Germany — [2]NewTechnologies-Research Center, University of West Bohemia, Pilsen, Czech Republic

The Korringa-Kohn-Rostoker-Green function (KKR-GF) method provides a very suitable platform to describe the electronic structure of iron pnictide superconducting compounds with substitutional disorder. [1] Having direct access to the Green function allows in a rather straightforward manner to perform calculations on angle-resolved photoemission spectroscopy (ARPES). This can be done on the basis of the one-step model of photoemission leading to results that can be directly compared to experimental ARPES data, unveiling significantly more information than pure band structure calculations. Corresponding ARPES calculations have been done with a focus on the strong in-plane anisotropy in antiferromagnetic $BaFe_2As_2$ and its evolution under Co substitution in $Ba(Fe_{1-x}Co_x)_2As_2$. The resulting ARPES spectra are discussed in comparison with experimental ARPES data measured on detwinned crystals. [2] In particular it is demonstrated that the variation of the electronic structure with Co substitution as monitored by ARPES is well reproduced by theory.

[1] G. Derondeau *et al.*, Phys. Rev. B **90**, 184509 (2014).
[2] M. Yi *et al.*, PNAS **108**, 6878 (2011).

TT 79.10 Thu 18:00 H21

High field properties of superconducting $BaFe_{2-x}Ni_xAs_2$ thin films — •Stefan Richter[1,2], Fritz Kurth[1], Kazumasa Iida[3], Vadim Grinenko[1], Kirill Pervakov[4], Chiara Tarantini[5], Jan Jaroszynski[5], Aurimas Pukenas[2], Werner Skrotzki[2], Kornelius Nielsch[1], and Ruben Hühne[1] — [1]Institute for Metallic Materials IFW Dresden — [2]Technical University Dresden — [3]Nagoya University, Japan — [4]Russian Academy of Sciences, Russia — [5]National High Magnetic Field Laboratory, USA

Fe based superconductors combine the advantages of cuprates (high upper critical field) with the small Hc_2 anisotropy of classic low temperature superconductors, which makes them suitable candidates for high field applications. The study of Fe-based superconducting thin films is one crucial step to explore this potential in more detail.

We present results for epitaxial $BaFe_{2-x}Ni_xAs_2$ thin films, which have been successfully grown for the first time using pulsed laser deposition. Superconducting transition temperatures of up to 19 K have been realized in slightly overdoped films, which is in good agreement with results obtained for single crystals. The behavior of the upper critical field and critical current density has been measured in high magnetic fields up to 35 T. The results will be correlated to the observed microstructure and compared to high field data for single crystals with similar composition.

Funding of this work by DFG GRK 1621 is gratefully acknowledged.

TT 79.11 Thu 18:15 H21

Electrical transport properties of the unconventional superconductor YFe_2Ge_2 — •Konstantin Semeniuk[1], Jiasheng Chen[1], Zhuo Feng[2], Philip Brown[1], Yang Zou[1], Giulio Lampronti[3], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge UK — [2]London Centre of Nanotechnology, University College London, London UK — [3]Dept. of Earth Sciences, University of Cambridge, Cambridge UK

YFe_2Ge_2 is a paramagnetic d-electron system which stands out due to its high Sommerfeld ratio of its specific heat capacity of 100 mJ/(mol K^2) and non Fermi-liquid $T^{3/2}$ power law temperature dependence of the electrical resistivity. The material was found to be superconducting below about 1.8 K [1].

Advances in YFe_2Ge_2 crystal growth allowed us to obtain high quality samples with residual resistivity ratios of the order of 200. Recent measurements of magnetisation and heat capacity provide further evidence for superconductivity, and the correlation between the transition temperature and the sample quality, the enhanced Sommerfeld coefficient and the anomalous T-dependence of the resistivity indicate that superconductivity in YFe_2Ge_2 is unconventional [2]. We report the results of detailed electrical resistivity measurements on YFe_2Ge_2 as a function of temperature, magnetic field and hydrostatic pressure, which provide further insight into the nature of superconducting and normal states of the material.

[1] Y. Zou et al., Physica Status Solidi (RRL) **8**, 928 (2014).
[2] J. Chen et al., arXiv:1507.01436v2.

TT 80: Correlated Electrons: (General) Theory 2

Time: Thursday 16:00–18:30 Location: H18

TT 80.1 Thu 16:00 H18

A novel solution of the Hubbard model: a generalized equation-of-motion approach to the underdoped cuprates puzzle — •Andrea Di Ciolo[1] and Adolfo Avella[1,2] — [1]Dipartimento di Fisica "E.R. Caianiello", Università degli Studi di Salerno, I-84084 Fisciano (SA), Italy — [2]CNR-SPIN, UoS di Salerno, I-84084 Fisciano (SA), Italy

We solve the Hubbard model on a d-dimensional hypercubic lattice in the framework of the Composite Operator Method (COM) within a 4-pole approximation. This approach extends the 2-pole [1] and the 3-pole [2] schemes treating on equal footing both U and J scales of energy. The COM, which is based on the Green's function formalism, is highly tunable and expressly devised for the characterization of strongly correlated electronic states and the exploration of novel emergent phases. Motivated by the long-standing experimental challenge posed by the puzzling spectral properties of the underdoped cuprates, we adopt a basis of fields containing operators specifically designed to describe Hubbard electronic transitions dressed by nearest-neighbor spin fluctuations and to capture the effects of these latter on all electronic properties. The spin fluctuations play a crucial role in the mechanism of pseudogap formation and evolution as well as in the unconventional behavior of the Fermi surface, the spectral weights and the electronic dispersion. Thus, we exploit this non canonical, but very efficient,

operatorial representation of correlated electrons to achieve a deeper understanding of the underdoped phase of cuprates.
[1] F. Mancini, and A. Avella, Adv. Phys. **53**, 537 (2004)
[2] A. Avella, Eur. Phys. J. B **87**, 45 (2014)

TT 80.2 Thu 16:15 H18

Multiplons in the two-hole excitation spectra of the Hubbard model — •Roman Rausch and Michael Potthoff — I. Institute for Theoretical Physics, University of Hamburg

Using the density-matrix renormalization group (DMRG) in combination with the Chebyshev polynomial expansion technique, we study the two-hole excitation spectra of the one-dimensional Hubbard model from $n = 2$ down to half-filling $n = 1$. Experimentally, this corresponds to the Auger Electron Spectroscopy (AES). The spectra reveal multiplon physics, i.e., the relevant final states are characterized by two (doublon), three (triplon), four (quadruplon) and more holes, potentially forming stable compound objects or resonances with finite lifetime. This multiplon phenomenology is analyzed by interpreting not only the local and k-resolved two-hole spectra, but also auxiliary three- and four-hole spectra, as well as by referring to effective low-energy models and employing a filter-operator technique. In addition, we compare with the elementary excitations of the Bethe ansatz, which in particular reveals the decay channels of the doublon into spinons and holons in one dimension. For all fillings with $n > 1$, the doublon lifetime is strongly k-dependent and even infinite at the Brillouin zone edges. This can be traced back to the "hidden" charge-SU(2) symmetry of the model. We briefly discuss how this k-dependence changes in two dimensions, by applying DMRG to small-radius cylinders, as well as extrapolating to larger systems by using cluster perturbation theory (CPT).
[1] R. Rausch, M. Potthoff, arXiv:1510.01162

TT 80.3 Thu 16:30 H18

Doping effects on the three-orbital spin-orbit-coupled Hubbard model — •Aaram J. Kim[1], Harald O. Jeschke[1], Philipp Werner[2], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany — [2]Department of Physics, University of Fribourg, Chemin du Musée 3, 1700 Fribourg, Switzerland

We investigate doping effects in a spin-orbit-coupled three-orbital Hubbard model by means of the dynamical mean-field theory combined with the continuous-time quantum Monte Carlo method. Near 5/6-filling, the spin-orbit-coupled Mott insulator emerges as a consequence of the interplay between the relativistic spin-orbit term and the strong U interaction. In particular, we discuss the spectral properties of the hole-doped spin-orbit-coupled Mott insulator and its phase transitions as a function of interaction U and doping concentration. The two-particle correlation function is also studied to show the dynamic properties of the system. We discuss implications of the model results for real materials.

TT 80.4 Thu 16:45 H18

Hybrid-Space Density Matrix Renormalization Group applied to the Two-Dimensional Hubbard Model — •Georg Ehlers and Reinhard M. Noack — Philipps-University Marburg

We apply the hybrid-space density matrix renormalization group (DMRG) to the two-dimensional Hubbard model on a cylinder surface. The hybrid-space DMRG uses a momentum-space representation in the transverse and a real-space representation in the longitudinal direction. Utilizing the transverse momentum quantum number allows us to gain significant speedup and memory savings compared to real-space DMRG. Especially, the computational costs of the hybrid-space DMRG are almost independent of the cylinder circumference for fixed size of the truncated Hilbert space. We investigate ground state properties such as the behavior of the ground-state energy, pair-field correlations, and the appearance of stripes at intermediate coupling and weak doping. We find striped ground states generically, with the width of the stripes depending on the filling, the boundary conditions, and the width of the cylinder. Furthermore, we analyze the interplay between the different stripe configurations and the decay of the pairing correlations.

15 min. break

TT 80.5 Thu 17:15 H18

Ground state phase diagram of the repulsive fermionic t-t' Hubbard model on the square lattice from weak-coupling — •Fedor Simkovic[1], Xuan-Wen Liu[2], Youjin Deng[2], and Evgeny Kozik[1] — [1]King's College London, Strand, London WC2R 2LS, UK — [2]University of Science and Technology of China, Hefei, Anhui 230026, China

We obtain a complete and exact in the weak-coupling limit ($U \to 0$) ground state phase diagram of the repulsive fermionic Hubbard model on the square lattice for filling factors $0 \leq n \leq 2$ and next nearest neighbour hopping amplitudes $0 \leq t' \leq 0.5$. Phases are distinguished by the symmetry and the number of nodes of the superfluid order parameter. The phase diagram is richer than may be expected and typically features states with a high —higher than that of the fundamental mode of the corresponding irreducible representation— number of nodes. The effective coupling strength in the Cooper channel λ, which determines the critical temperature T_c of the superfluid transition, is calculated in the whole parameter space and regions with high values of λ are identified. It is shown that besides the expected increase of λ near the Van Hove singularity line, joining the ferromagnetic and antiferromagnetic points, another region with high values of λ can be found at quarter filling and $t' = 0.5$ due to the presence of a line of nesting at $t' \geq 0.5$. The results can serve as benchmarks for controlled non-perturbative methods and guide the ongoing search for high-T_c superconductivity in the Hubbard model.

TT 80.6 Thu 17:30 H18

Nature of the many-body excitations in a quantum wire — •Oleksandr Tsyplyatyev — Institut für Theoretische Physik, Universität Frankfurt, Frankfurt, Germany

The natural excitations of an interacting one-dimensional system at low energy are hydrodynamic modes of Luttinger liquid, protected by the Lorentz invariance of the linear dispersion. We show that beyond low energies, where quadratic dispersion reduces the symmetry to Galilean, the main character of the many-body excitations changes into a hierarchy: calculations of dynamic correlation functions for fermions (without spin) show that the spectral weights of the excitations are proportional to powers of R^2/L^2, where R is a length-scale related to interactions and L is the system length. Thus only small numbers of excitations carry the principal spectral power in representative regions on the energy-momentum planes. We have analysed the spectral function in detail and have shown that the first-level (strongest) excitations form a mode with parabolic dispersion, like that of a renormalised single particle. The second-level excitations produce a singular power-law line shape to the first-level mode and multiple power-laws at the spectral edge. We have illustrated crossover to Luttinger liquid at low energy by calculating the local density of state through all energy scales: from linear to non-linear, and to above the chemical potential energies.
[1] O. Tsyplyatyev et al., PRL **114**, 196401 (2015).
[2] O. Tsyplyatyev et al., arXiv:1508.07125.

TT 80.7 Thu 17:45 H18

Theoretical calculation of photoemission spectra for Ir-based perovskites — •Ekaterina Plotnikova[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, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland — [3]University of British Columbia, 6224 Agricultural Road, Vancouver, BC V6T 1Z1 Canada

The layered iridates, Ba_2IrO_4 and Sr_2IrO_4, have recently attracted a lot of attention due to their structural and electronic similarities to the layered cuprates. Nevertheless, due to the strong spin-orbit coupling in the iridates, their properties upon electron or hole doping *may* be substantially different than those of the high-T_C cuprates. As a first step in understanding the physics of the doped iridates, we calculate the photoemission spectra of layered iridates using a polaronic model and the self-consistent Born approximation. We compare the obtained spectra to those calculated using the density functional theory and to the experimental spectra obtained by ARPES on Ba_2IrO_4 and Sr_2IrO_4.

TT 80.8 Thu 18:00 H18

The shape of the Compton profile for metals — •Michael Sekania[1,2], Wilhelm H. Appelt[1,3], Diana Benea[4,5], Hubert Ebert[5], 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 — [4]Faculty of Physics, Babes-Bolyai University, Kogalniceanustr 1, Ro-400084 Cluj-Napoca, Romania and — [5]Department of Chemistry, Ludwig Maximilian University of Munich, Butenandstr. 5-13, D-81377 München, Germany

The electron momentum density and Compton profiles of weakly interacting metals are investigated in the framework of the density functional theory. The valence electrons contributions to the Compton profiles for different lattice symmetries are analyzed. We find that the shape of the Compton profiles can be modeled by the so-called q-Gaussian distribution recently proposed by Tsallis in the context of generalized canonical distributions. Our analysis shows that tails typically ignored in the conventional studies of the Compton profiles contain significant information about the electron momentum distribution in solids.

TT 80.9 Thu 18:15 H18

Rigorous Bounds on Pomeranchuk $l = 1$ Instabilities from Ward Identities — •Egor Kiselev[1], Mathias Scheurer[1], Jörg Schmalian[1,2], and Peter Wölfle[1,3] — [1]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology, 76049 Karlsruhe, Germany — [2]Institute for Solid State Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [3]nstitut für Nanotechnologie, Karlsruher Institut für Technologie, D-76021 Karlsruhe, Germany

Pomeranchuk Instabilities signal spontaneous deformations of the Fermi surface. The shape of those deformations is parametrized by spherical harmonics $Y_{l,0}$, so that Pomeranchuk Instabilities can be classified by the number l. In the $l = 1$ case the Fermi surface is displaced by a small momentum and the instability results in spontaneously flowing spin or charge currents.

Using generalized Ward Identities it will be shown, that $l = 1$ Pomeranchuk Instabilities in the spin/charge sector cannot be caused by a locally spin/charge conserving interaction respectively. Since the general case of Coulomb interaction between electrons and ions conserves electronic spin and charge, it is concluded that $l = 1$ Pomeranchuk Instabilities can only occur, when relativistic physics is considered.

We discuss implications of our results for proposed emergent spin-orbit couplings, preemptive Pomeranchuk Instabilities near a ferromagnetic quantum critical point, and the low temperature Fermi liquid behaviour of ^{3}He.

TT 81: Transport: Spintronics and Magnetotransport (Joint session of DS, HL, MA and TT organized by TT)

Time: Thursday 16:15–18:30 Location: H23

Invited Talk TT 81.1 Thu 16:15 H23

Non-Abelian gauge theory description of (dynamical) spin-orbit coupling effects in Fermi gases. — •Cosimo Gorini — Institut für Theoretische Physik, Universität Regensburg, Germany

Spin-orbit coupling heavily influences the dynamics of charge carriers in a solid, where its strength can be enhanced by orders of magnitude as compared to the vacuum. Remarkable consequences are phenomena such as the spin Hall and inverse spin galvanic (or Edelstein) effects, where spin currents and polarizations are generated by purely electrical means. The intricacies of such rich spin-charge coupled dynamics can be described within a non-Abelian gauge theory approach [1], based on Keldysh non-equilibrium formalism [2]. Thanks to a symmetric treatment of spin and charge degrees of freedom, and the removal of ambiguities related to spin non-conservation in the presence of (static or dynamical) spin-orbit coupling, a physically transparent picture is achieved [3]. Furthermore, the non-Abelian language, by virtue of its universal character, treats on the same footing standard spin-orbit interaction in solid state systems and exotic forms of (pseudo) spin-orbit coupling which arise, or can be engineered, in different contexts.

[1] H. Mathur and A. D. Stone, PRL **68**, 2964 (1991)
I. V. Tokatly, PRL **101**, 106601 (2008).
[2] C. Gorini et al., PRB **82**, 195316 (2010).
[3] C. Gorini et al., PRL **109**, 246604 (2012)
C. Gorini et al., PRL **115** , 076602 (2015).

TT 81.2 Thu 16:45 H23

Shot noise in magnetic tunnel junctions: effect of the geometric phase — •Tim Ludwig[1] and Alexander Shnirman[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]L. D. Landau Institute for Theoretical Physics RAS, Kosygina street 2, 119334 Moscow, Russia

We analyze the current driven dynamics of magnetization and voltage in a magnetic tunnel junction. As predicted in [1, 2], the magnetization can be driven by spin currents. This effect can also be reversed, such that an externally driven magnetization generates a dc voltage [3]. Although both effects are intimately related, so far they have been treated separately. We generalize the approach of [4] to derive an action that contains both effects simultaneously. We employ the Keldysh formalism, which allows us to derive stochastic Landau-Lifshitz-Gilbert-Langevin equations describing the angular dynamics of the magnetization coupled with the voltage dynamics. We identify two low-temperature regimes. In one regime the voltage fluctuations are governed by the applied current only, as expected for the shot noise. In the other regime an excess noise arises, which is governed by the geometric phase of the precessing magnetization.

[1] L. Berger, PRB **54**, 9353 (1996)
[2] J. C. Slonczewski, J. Magn. Magn. Mater. **159**, L1 (1996)
[3] L. Berger, PRB **59**, 11465 (1998)
[4] A. Shnirman, Y. Gefen, A. Saha, I. S. Burmistrov, M. N. Kiselev, A. Altland, PRL **114**, 176806 (2015)

TT 81.3 Thu 17:00 H23

Electron transport through the helical molecules in the presence of spin-orbit coupling — •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 it was shown [1] that electron transport through systems with helical symmetry shows spin selectivity. Here we present a theoretical investigation of the transport properties through helical molecules placed between magnetic and nonmagnetic leads by using the DFT and NEGF approach. The performed analysis of the data allow us to show that the systems show spin-polarization only because of spin-orbit interaction and the spin polarization is clearly related to the helical symmetry since a change in handedness of the helix changes the sign of the spin-polarization and a linear chain does not display any sizeable polarization.

[1] B. Göhler, V. Hamelbeck, T. Z. Markus, M.Kettner, G. F. Hanne, Z. Vager, R. Naaman, and H. Zacharias, Science **331**, 894 (2011).

15 min. break

TT 81.4 Thu 17:30 H23

Magnetic impurities on Bi thin films - conductivity and surface diffusion — •Philipp Kröger[1], Sergii Sologub[2], Andreas Lücke[3], Nora Vollmers[3], Uwe Gerstmann[3], Wolf Gero Schmidt[3], Herbert Pfnür[1], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Inst. für FKP, Appelstr. 2, 30167 Hannover — [2]Inst. of Ph., Nat. Acad. of Sc., Nauky Av. 46, 03028 Kyiv, Ukraine — [3]Universität Paderborn, Theoretische Materialphysik, Pohlweg 55, 33098 Paderborn

The semimetal bismuth has attracted a lot of interest because of its unique electronic properties such as low carrier concentration and large mobility. The surface states reveal a pronounced Rashba splitting. The surface conductivity can well be discriminated from bulk contributions for ultra-thin films grown epitaxially on Si(111) substrates, so that surface related effects are accessible even in macroscopic conductance measurements.

In this context, the adsorption of Cr with its high magnetic moment on the Bi(111) surface will be discussed. Cr induces a transition from Weak Anti- to Weak Localization. This indicates strong impurity scattering that mixes spin and orbit momenta, with corresponding symmetry breaking on the Bi surface (TRS), in agreement with results from

DFT calculations. Contrary to other impurities adsorbed at subsurface sites (Fe,Co,Cr, Sb), Cr shows signs of diffusion processes at low T (T ≈ 10 K), as previously observed for Tb which adsorbes on the surface.

TT 81.5 Thu 17:45 H23

Spin-vibronics in interacting nonmagnetic molecular nanojunctions — •Stephan Weiss[1], Jochen Brüggemann[2], and Michael Thorwart[2] — [1]Theoretische Physik, Universität Duisburg-Essen & CENIDE — [2]1. Institut für Theoretische Physik, Universität Hamburg

We show that in the presence of ferromagnetic electronic reservoirs and spin-dependent tunnel couplings, molecular vibrations in nonmagnetic single molecular transistors induce an effective intramolecular exchange magnetic field[1]. It generates a finite spin-accumulation and -precession for the electrons confined on the molecular bridge and occurs under (non)equilibrium conditions. The effective exchange magnetic field is calculated here to lowest order in the tunnel coupling for a nonequilibrium transport setup. Coulomb interaction between electrons is taken into account as well as a finite electron-phonon coupling. For realistic physical parameters, an effective spin-phonon coupling emerges. It is induced by quantum many-body interactions, which are either electron-phonon or Coulomb-like.

[1] S. Weiss, J. Brüggemann and M. Thorwart, PRB **92**, 045431 (2015).

TT 81.6 Thu 18:00 H23

Coherent Dynamics of Quantum Spins in Magnetic Environments — •Lars-Hendrik Frahm[1], Christoph Hübner[1], Benjamin Baxevanis[1,2], and Daniela Pfannkuche[1] — [1]1. Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg, Germany — [2]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands

We investigate equilibration and transport effects of a magnetic atom that is exchange coupled to two electron reservoirs. An effective crystal field, which arises from the substrate the atom is living on gives the spin of the atom an easy axis for alignment. Further, a spin-polarized electron reservoir breaks the rotation symmetry around the spin quantization axis. A proper description of the dynamics of the quantum spin requires to consider the complete density operator, where its knowledge allows to calculate magnetization dynamics and transport properties on an equal footing. We discuss the electron transport through the atomic system by especially focusing on the non-linear influence of the spin torque effect.

TT 81.7 Thu 18:15 H23

Colossal Magnetoresistance observed in Natural Graphite — •Jose Barzola-Quiquia[1], Mahsa Zoraghi[1], Markus Stiller[1], Christian Precker[1], Ana Champi[2], and Pablo Esquinazi[1] — [1]Institute for Experimental Physics II, University of Leipzig, 04103 Leipzig, Germany — [2]Centro de Ciencias Naturais e Humanas Universidade Federal do ABC, Sao Paulo- Brasil

In this work, the electrical transport properties of a bulk natural graphite flake extracted from a mine in Brazil were investigated. The sample showed metallic behavior and the changes in the magnetoresistance (MR) at 5 K and 7 T shows 1123600% change when the field was applied parallel to the *c*-axis. This value was not yet reported in any graphite sample in the literature. Applying constant magnetic field, resistance measurements as a function of the temperature show also a magnetic field induces metal-insulator transition (MIT), with a small critical field $B_0 \approx 10$ mT compared to literature. We observed also that at fields B > 0.2 T a metallic reentrance was observed that remains up to ≈ 50 K. STEM measurements reveal the presence of interfaces in the investigated material. Therefore, the observed transport properties are not an intrinsic behavior of the graphite sample but due to the presence of these interfaces. Interfaces in the sample are formed at the interfaces between two crystalline regions inside the sample where a two dimensional electron gas (2DEG) system appears. Raman measurements reveal that our samples are free from any other defects.

TT 82: Correlated Electrons: Nonequilibrium Quantum Many-Body Systems 2

Time: Thursday 16:30–18:30 Location: H22

TT 82.1 Thu 16:30 H22

Dynamical Cooper pairing in non-equilibrium electron-phonon systems — •Michael Knap[1,2], Mehrtash Babadi[3], Gil Refael[3], Ivar Martin[4], and Eugene Demler[2] — [1]Technical University of Munich — [2]Harvard University — [3]Caltech — [4]Argonne National Laboratory

Ultrafast laser pulses have been used to manipulate complex quantum materials and to induce dynamical phase transitions. One of the most striking examples is the transient enhancement of superconductivity in several classes of materials upon irradiating them with high intensity pulses of terahertz light. Motivated by these experiments we analyze the Cooper pairing instabilities in non-equilibrium electron-phonon systems. We demonstrate that the light induced non-equilibrium state of phonons results in a simultaneous increase of the superconducting coupling constant and the electron scattering. We analyze the competition between these effects and show that in a broad range of parameters the dynamic enhancement of Cooper pair formation dominates over the increase in the scattering rate. This opens the possibility of transient light induced superconductivity at temperatures that are considerably higher than the equilibrium transition temperatures. Our results pave new pathways for engineering high-temperature light-induced superconducting states.

TT 82.2 Thu 16:45 H22

Non-Equilibrium Dynamical Cluster Approximation of the Falicov-Kimball Model — •Andreas Herrmann and Philipp Werner — University of Fribourg, Switzerland

We simulate the time-evolution of the Falikov-Kimball model after an interaction quench using a non-equilibrium generalization of the dynamical cluster approximation (DCA). By considering clusters of up to eight sites, we study how non-local correlations affect the relaxation dynamics of local and non-local observables.

TT 82.3 Thu 17:00 H22

Fluctuations of the entanglement entropy in strongly disordered systems — •Johannes Oberreuter and Michael Knap — Walter-Schottky-Institut, Technische Universität München, Garching, Deutschland

The fact that disorder localizes the dynamics in one- and two-dimensional systems is a classic result by Anderson. Recently, the question has arisen, if this effect also pertains to quantum many body systems with interactions, which is known as many body localization (MBL). It has been suggested, that the fluctuations of the entanglement entropy could provide a signature of MBL. We examine this quantity in the framework of the strong randomness (real space) renormalization group. We compare numerical simulations and analytical findings in the infinite randomness fixed point.

TT 82.4 Thu 17:15 H22

Scaling and Universality at Dynamical Quantum Phase Transitions — •Markus Heyl — Technische Universität München

Dynamical quantum phase transitions have recently emerged as a nonequilibrium analogue to conventional phase transitions with physical quantities becoming nonanalytic at critical times. However, a major challenge is to connect to fundamental concepts such as scaling and universality that are intimately related to renormalization group theory and the associated fixed points. In this talk I will show that for dynamical quantum phase transitions in Ising models exact renormalization group transformations in complex parameter space can be formulated. As a result of this construction, the dynamical quantum phase transitions are critical points associated with unstable fixed points of equilibrium Ising models implying scaling and universality. Moreover, signatures of these transitions in the dynamical buildup of spin correlations will be presented with an associated temporal power-law scaling determined solely by the fixed point universality class.

TT 82.5 Thu 17:30 H22

Non-equilibrium inhomogeneous DMFT for correlated Het-

erostructures: Auxiliary Master Approach — •Irakli Titvinidze, Antonius Dorda, Wolfgang von der Linden, and Enrico Arrigoni — Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

The recent impressive experimental progress in tailoring different microscopically controlled quantum objects has prompted increasing interest in correlated systems out of equilibrium. Of particular importance are correlated heterostructures, quantum wires and quantum dots with atomic resolution. In this work we present results for the steady state spectral function and current-voltage characteristics for a system consisting of several monoatomic layers of correlated orbitals, attached to two metallic leads. The non-equilibrium situation is driven by a bias-voltage applied to the leads. To investigate the system we generalize a recently introduced dynamical mean-field theory (DMFT) based theoretical scheme [1] for the multilayer case. Specifically, the approach addresses the DMFT 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 [1,2,3].

[1] E. Arrigoni et al., PRL **110**, 086403 (2013)
[2] A. Dorda et al., PRB **89**, 165105 (2014)
[3] I. Titvinidze et al., arxiv:1508.02953

TT 82.6 Thu 17:45 H22

Quasi-soliton scattering in quantum spin chains — •Davide Fioretto[1], Rogier Vlijm[2], Martin Ganahl[3], Michael Brockmann[4], Masud Haque[4], Hans-Gerd Evertz[5], and Jean-Sébastien Caux[2] — [1]Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1090 GL Amsterdam, The Netherlands — [3]Perimeter Institute for Theoretical Physics, 31 Caroline Street North, ON N2L 2Y5, Canada — [4]Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Strasse 38, 01187 Dresden, Germany — [5]Institut für Theoretische Physik, Technische Universität Graz, Petersgasse 16, 8010 Graz, Austria

The quantum scattering of magnon bound states in the anisotropic Heisenberg spin chain is shown to display features similar to the scattering of solitons in classical exactly solvable models. Localized colliding Gaussian wave packets of bound magnons are constructed from string solutions of the Bethe equations and subsequently evolved in time, relying on an algebraic Bethe ansatz based framework for the computation of local expectation values in real space-time. The local magnetization profile shows the trajectories of colliding wave packets of bound magnons, which obtain a spatial displacement upon scattering. Analytic predictions on the displacements for various values of anisotropy and string lengths are derived from scattering theory and Bethe ansatz phase shifts, matching time evolution fits on the displacements.

TT 82.7 Thu 18:00 H22

Electron-phonon scattering in one-dimensional systems — •Christoph Brockt[1], Eric Jeckelmann[1], Florian Dorfner[2], Lev Vidmar[2], and Fabian Heidrich-Meisner[2] — [1]Leibniz Universität Hannover, Germany — [2]Ludwig-Maximilians-Universität München, Germany

We present a study of the scattering of an electronic wave packet by local phonon modes on an one-dimensional lattice. The problem is adressed both numerically and analytically. We find features like transient self-trapping, reflection and dissipation, where the latter two exhibit resonance effects. The parameter range includes the adiabatic, antiadiabatic, weak- and strong coupling regimes. For the numerical part we use a newly developed method for simulating the time evolution of systems with large local Hilbert spaces [1]. It combines the time-evolving block-decimation algorithm [2] with a dynamical optimization of the local boson basis. We use the optimal boson modes [3] to speed up our simulations as well as for gaining insight into the physics of the system.

Support from the DFG through the Research Unit FOR 1807 is gratefully acknowledged.

[1] C. Brockt et al., arXiv:1508.00694v1 (2015)
[2] G. Vidal, PRL **93**, 040502 (2004)
[3] C. Zhang, E. Jeckelmann, and S. R. White, PRL **80**, 2661 (1998)

TT 82.8 Thu 18:15 H22

Filling fraction quantum quenches and the arctic circle — •Jean-Marie Stephan[1], Jacopo Viti[1], Jerome Dubail[2], Nicolas Allegra[2], and Masud Haque[1] — [1]Max Planck Institut für Physik Komplexer Systeme, Noethnitzer Str. 38 D01187 Dresden, Germany — [2]CNRS & IJL-UMR 7198, Universite de Lorraine, BP 70239, F-54506 Vandoeuvre-les-Nancy Cedex, France

I consider a simple non-equilibrium problem, where a critical one-dimensional system is prepared in a state with two different densities on the left and on the right, and let evolve with a Hamiltonian that conserves the number of particles. For free systems a lot can, and has been understood by making use of a semiclassical picture, in which particles carrying a momentum k propagate ballistically with velocity v(k). Generalization to interacting systems is very much an open problem. I will discuss attempts at understanding such dynamics using field theory. A possible strategy is to study the behavior in imaginary time, the real time dynamics being recovered by performing the Wick rotation. I will show that all degrees of freedom outside a certain region may freeze in imaginary time, contrary to naive expectations. This behavior is analogous to the celebrated "arctic circle" phenomenon found in the study of two-dimensional classical dimer or vertex models. Such imaginary time pictures can be used to make predictions about the behavior of correlation functions, entanglement entropies, or return probabilities after the quench.

TT 83: Symposium on Frontiers of Electronic Structure Theory: Focus on Topology and Transport (SYES)
(Joint symposium of DS, HL, MA, MM, O and TT organized by O)

Time: Friday 9:30–12:15 Location: H1

Invited Talk TT 83.1 Fri 9:30 H1

Intrinsic Transport Coefficients and Momentum Space Berry Curvatures — •Allan H MacDonald — University of Texas at Austin, Austin TX, USA

The response of a conductor to a bias voltage is normally dominated by repopulation of states near the Fermi level. The transport steady state is fixed by a competition between acceleration in an electric field and disorder-induced scattering which attempts to restore equilibrium. This response of observables to a bias voltage is therefore extrinsic. There is however also response of states away from the Fermi level, which are polarized by the electric field. Provided that the typical band separation is larger than the finite life-time uncertainty in Bloch state energies this response is intrinsic, and for some observables it can be dominant. Intrinsic response coefficients are attractive targets for electronic structure theory because they are readily evaluated. Examples of responses to bias voltages that are sometimes dominantly intrinsic are the anomalous Hall conductivity of ferromagnetic or antiferromagnetic conductors, the spin-Hall conductivity of heavy metals, and current-induced torques in heavy-metal/ferromagnet systems. Intrinsic transport coefficients tend to be large in crystals with large momentum-space Berry curvatures, for example in crystals with topologically non-trivial electronic structure, and remain finite when a gap opens at the Fermi level to eliminate the Fermi surface. I will discuss some important examples of transport coefficients that are dominated by intrinsic contributions, mentioning as an important case the quantum anomalous Hall effect.

Invited Talk TT 83.2 Fri 10:00 H1

Berry phase linked spin-orbit torques in Ferromagnetic and Antiferromagnetic systems — •Jairo Sinova — Johannes Gutenberg Universität Mainz, Staudingerweg 7, 55128 Mainz Germany

As current-driven torques are becoming more relevant in future MRAM technologies, in-plane current magnetization dynamics driven by the so called Rashba spin-orbit torques or through a combination of spin-Hall effect and spin-transfer torque has become more and more important. Understanding these torques is paramount to maximize their

use. In recent experiments we have shown that in addition to the intrinsic SHE and STT effect there exists an intrinsic spin-orbit torque originating from the Berry phase of the spin-orbit coupled Bloch electrons analogous to the intrinsic spin Hall effect. This type of torques can be observed through SO-FMR driven experiments. We show this new type of toques in theory and experiments in GaMnAs and show that it can be of similar strength to the strong field-like torque. In addition, we extend these physics to a new type of order-parameter manipulation by currents by examining the combined effect of spin-orbit coupling and anti-ferromagnetic order. We show that in broken inversion symmetry anti-ferromagnets a current will induced a non-equilibrium Néel-order field that will act directly on the Néel order parameter, hence making the direct manipulation of anti-ferromagnets without auxiliary exchange biased coupling to other ferromagnets a new and exciting possibility. One of these type of Néel torques has been recently experimentally confirmed.

Invited Talk TT 83.3 Fri 10:30 H1

Transport in Topological Insulators and Topological Superconductors: In Search of Majorana Fermions — •Ewelina Hankiewicz — Wuerzburg University

Topological insulators (TIs) have a bulk energy gap that separates the highest occupied band from the lowest unoccupied band and the metallic gapless states at the edge [1]. Similarly, topological superconductors (TSC) have gapless zero energy states protected by the particle-hole symmetry, which in some cases form Majorana bound states. Here, we focus on the proximity-induced superconductivity in TIs [2] as well as on unusual properties of TSC [3] showing that they both can pave a road to find a Majorana state.

Concerning proximity-induced superconductivity in TIs, we describe a novel superconducting quantum spin-Hall effect, which is protected against elastic backscattering by combined time-reversal and particle-hole symmetry even in magnetic fields [2]. We discuss unusual transport properties of this effect and possible Majorana detection schemes.

Finally, we discuss new systems like TSC on the hexagonal lattices. We develop combined microscopic and macroscopic description of these materials that predicts realistic scanning tunneling microscopy signal in these superconductors [3]. Is there a way to measure Majorana state in these systems?

[1] G. Tkachov and E. M. Hankiewicz, Review in Phys. Status Solidi B 250, 215 (2013). [2] R. Reinthaler, G. Tkachov and E.M. Hankiewicz, Phys. Rev. B 92, 161303(R) (2015). [3] L. Elster, C. Platt, R. Thomale, W. Hanke, and E. M. Hankiewicz, Nature Comm. 6, 8232 (2015).

session break

Invited Talk TT 83.4 Fri 11:15 H1

Engineering Topological Quantum States: From 1D to 2D. — •Jelena Klinovaja — University of Basel, Switzerland

I will discuss low-dimensional condensed matter systems, in which topological properties could be engineered per demand. Majorana fermions can emerge in hybrid systems with proximity pairing in which the usually weak Rashba spin-orbit interaction is replaced by magnetic textures. I will discuss candidate materials such as semiconducting nanowires [1] and atomic magnetic chains [2]. One further goal is to go beyond Majorana fermions and to identify systems that can host quasiparticles with more powerful non-Abelian statistics such as parafermions in double wires coupled by crossed Andreev reflections [3,4]. Next, I will focus on 'strip of stripes model' consisting of weakly coupled one-dimensional wires [5-7], where interaction effects in the wires can be treated non-perturbatively via bosonization. Such systems can exhibit the integer or fractional quantum Hall effect, spin Hall effect, and anomalous Hall effect.

[1] J. Klinovaja and D. Loss, Phys. Rev. B 86, 085408 (2012). [2] J. Klinovaja, P. Stano, A. Yazdani, and D. Loss, Phys. Rev. Lett. 111, 186805 (2013). [3] J. Klinovaja and D. Loss, Phys. Rev. B 90, 045118 (2014). [4] J. Klinovaja, A. Yacoby, and D. Loss, Phys. Rev. B 90, 155447 (2014). [5] J. Klinovaja and D. Loss, Phys. Rev. Lett. 111, 196401 (2013); J. Klinovaja and D. Loss, Eur. Phys. J. B 87, 171 (2014). [6] J. Klinovaja and Y. Tserkovnyak, Phys. Rev. B 90, 115426 (2014). [7] J. Klinovaja, Y. Tserkovnyak, and D. Loss, Phys. Rev. B 91, 085426 (2015).

Invited Talk TT 83.5 Fri 11:45 H1

Skyrmions – Topological magnetization solitons for future spintronics — •Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Ultrathin magnetic films and heterostructures provide a fantastic playground for the stabilization, manipulation and usage of chiral magnetic skyrmions – topological magnetization solitons – magnetic entities described by a micromagnetic energy functional with particle like properties that may open a new vista for spintronics. A crucial quantity for the chiral skyrmion formation is the Dzyaloshinskii-Moriya interaction (DMI), whose presence in thin films could be established in a concerted effort of first-principles theory and spin-polarized scanning tunneling microscopy. It could be shown that the spin-orbit interaction and the structure inversion-asymmetry in these systems result in a DMI that is strong enough to give rise to one- and two-dimensional lattices of chiral spin-textures, chiral domain walls and even single skyrmions. In retrospect, it is surprising how little is known about the DMI in these metallic systems. In this talk I give insight into the DMI, relating first-principles calculations to different models, discussing the transport properties of electrons *e.g.* the topological (THE) and anomalous (AHE) Hall effect in relation to the spin texture of a skyrmion, and discuss possibilities to tailor the magnetic interactions to enlarge the materials base to stabilize single skyrmions. – I acknowledge fruitful collaborations with D. Crum, J. Bouaziz, B. Dupé, S. Heinze, N. Kiselev, S. Lounis, Y. Mokrousov, A. Nandy, and B. Zimmermann.

TT 84: Topological Insulators II (Joint session of DS, HL, MA, O and TT organized by O)

Time: Friday 9:30–12:00 Location: H15

TT 84.1 Fri 9:30 H15

Signatures of induced superconductivity in a p-n heterostructure comprised of Sb_2Te_3 and Bi_2Te_3 3D topological insulator thin films with in situ Al capping — •Peter Schüffelgen[1], Daniel Rosenbach[1], Martin Lanius[1], Jörn Kampmeier[1], Gregor Mussler[1], Markus Eschbach[1], Ewa Mlynczak[1], Lukasz Plucinski[1], Martina Luysberg[1], Stefan Trellenkamp[1], Martin Stehno[2], Prosper Ngabonziza[2], Alexander Brinkman[2], Yuan Pang[3], Li Lu[3], Thomas Schäpers[1], and Detlev Grützmacher[1] — [1]Peter Grünberg Institut and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]TNW and MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands — [3]Laboratory for Solid State Quantum Information and Computation, Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China

We investigate the transport properties of Sb_2Te_3/Bi_2Te_3 p-n heterostructure topological insulator film-superconductor junctions. The films are 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 Dirac-like surface states. Josephson junctions are defined by depositing two niobium electrodes, separated by a few tens of nanometers, onto the Sb_2Te_3/Bi_2Te_3 layer. The transport measurements at cryogenic temperatures showed signatures of Andreev reflections and Josephson supercurrents. For wider junctions a Fraunhofer pattern was observed for the critical current, whereas for the narrow junctions a monotonous decrease was found.

TT 84.2 Fri 9:45 H15

Teraherz-Induced Chiral Edge Photogalvanic currents in 2D HgTe Topological Insulators — •Kathrin-Maria Dantscher[1], Dimitry A. Kozlov[2], Maria-Theresia Scherr[1], Sebastian Gebert[1], Vasily V. Bel'kov[3], Nikolay N. Mikhailov[2], Sergey A. Dvoretskii[2], Ze Dong Kvon[2], and Sergey D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Institute of Semiconductor Physics, Novosibirsk, Russia — [3]Ioffe Institute, St. Petersburg, Russia

We report on the observation of a chiral photogalvanic current generated in the topological protected edge states of 2D topological insulators fabricated on the basis of 8 nm thick HgTe quantum wells. Illuminating the sample with circularly polarized terahertz radiation and picking-up the signal along the edges we detected a photocurrent whose direction reverses by switching radiation polarization from right- to left-handed one. The influence of the magnetic field, the temperature and the angle of incidence of the radiation to these photocurrents are investigated. We demonstrate that circularly polarized radiation, which, according to selection rules, excites only electrons with a certain spin, results in an imbalance of electron distribution in the k-space and causes a spin polarized electric current.

TT 84.3 Fri 10:00 H15

temperature induced shift of the chemical potential of Bi2Te2Se tetradymite topological insulators — •Jayita Nayak[1], Gerhard H Fecher[1], Siham Quardi[1], Chandra Sekhar[1], Claudia Felser[1], Christian Tusche[2], Shigenori Ueda[3], and Eiji Ikenaga[4] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden — [2]Max Planck Institute of Microstructure Physics, Halle — [3]Synchrotron X-ray Station at SPring-8National Institute for Materials Science, Hyogo 679-5148, Japan — [4]Japan Synchrotron Radiation Research Institute, SPring-8, Hyogo, 679-5198, Japan

The temperature dependent HAXPES spectra of Bi2Te2Se reveal the appearance of an additional spectral feature above the band gap at low temperature. It appears at 20 K but is absent in the 300 K spectra and the onset of the main features of the spectra is shifted to lower energies. Momentum resolved photoemission electron microscopy (k-PEEM)was carried out using in order to explain the origin of the additional spectral feature. The measurement provides the evidence of the evolution of bulk bands at low temperature which is caused by the shift of the chemical potential. The bulk sensitive HAXPES valence band spectra are in perfect agreement with first principles calculations.

TT 84.4 Fri 10:15 H15

Optical investigation of the three-dimensional Dirac semimetals $CaMnBi_2$ and $SrMnBi_2$ — •Micha B. Schilling[1], Artem V. Pronin[1], Martin Dressel[1], and Youguo Shi[2] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China

The interest in the measurements of optical conductivity in three-dimensional Dirac semimetals is based on the recent theoretical studies [1, 2], where the interband optical response of such systems has been shown to be very peculiar. Namely, the real part of the interband optical conductivity has been predicted to be linear in frequency with the slope being related to the Fermi velocity of Dirac electrons.

We investigated the optical properties of the three-dimensional Dirac semimetals $CaMnBi_2$ and $SrMnBi_2$ by means of Fourier-transform infrared spectroscopy. We measured the reflectivity over a frequency range from 50 to 25000 cm^{-1} at different temperatures down to 10 K and determined the optical conductivity from these measurements. In the presentation, we will discuss our results on the optical conductivity in comparison with theoretical predictions.

[1] P. Hosur, S. A. Parameswaran, and A. Vishwanath, Phys. Rev. Lett. **108**, 046602 (2012). [2] A. Bácsi and A. Virosztek, Phys. Rev. B **87**, 125425 (2013).

30 min. Coffee Break

TT 84.5 Fri 11:00 H15

Optoelectronic dynamics in nanocircuits based on the topological insulator Bi2Te2Se — •Mariana Hettich[1], Paul Seifert[1], Christoph Kastl[1], Kristina Vaklinova[2], Marko Burghard[2], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, D-85748 Garching, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

We report on the optoelectronic dynamics in nanocircuits made of the topological insulator Bi2Te2Se. An on-chip photocurrent pump-probe spectroscopy based on coplanar striplines allows us to identify the different ultrafast photocurrent mechanisms in topological insulators with a picosecond time resolution. We discuss non-equilibrium thermal effects as well as the circular photogalvanic current generation as contributions to the overall photocurrent.

TT 84.6 Fri 11:15 H15

Structural Study of Weak Topological Insulator Bi_1Te_1 Films on Si(111) grown by Molecular Beam Epitaxy — •Martin Lanius[1], Markus Eschbach[1], Ewa Mlynczak[1], Jens Kellner[2], Pika Gospodaric[1], Chengwang Niu[1], Elmar Neumann[1], Martina Luysberg[3], Gregor Mussler[1], Lukasz Plucinski[1], Gustav Bihlmayer[1], Stefan Blügel[1], Markus Morgenstern[2], Claus Michael Schneider[1], and Detlev Grützmacher[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [2]II. Institute of Physics B and JARA-FIT, RWTH Aachen University, Aachen, Germany — [3]Ernst Ruska-Centre for Microscopy and Spectroskopy with Electrons, Forschungszentrum Jülich, Germany

We have studied the nucleation, growth process and structural composition of the weak topological insulator Bi_1Te_1 on Si(111) substrates by STM and STEM. Bi_1Te_1 is a superlattice of predicted 2D topological insulating materials, one bilayer Bi and two Bi_2Te_3 quintuple layers per unit cell. The van der Waals growth mode of Bi_1Te_1 shows smooth surfaces and a supressed twin domain density. The thin films from several nanometers thickness down to the nucleation regime have been grown by molecular beam epitaxy. STEM measurements of the grown films reveal a high crystalline perfection. Simulations and ARPES measurements show 2D surface states originating from spin-orbit coupling, depending in their structure on the surface termination. Furthermore we will demonstrate the ability to grow n-p heterostructures of n-doped Bi_1Te_1 with the p-doped strong TI Sb_2Te_3.

TT 84.7 Fri 11:30 H15

Bi2Se3-based heterostructures including magnetic layers: the case of n-QLs Bi2Se3 ontop of Mn-doped Bi2Se3 — •J. Honolka[1], M. Valiska[2], J. Warmuth[3], M. Michiardi[4], M. Vondracek[1], A. S. Ngankeu[4], V. Holy[2], M. Bianchi[4], G. Springholz[5], V. Sechovsky[2], P. Hofmann[4], and J. Wiebe[3] — [1]Institute of Physics, ASCR, Prague, CZ — [2]Department of Condensed Matter, Charles University, Prague, CZ — [3]INF, University of Hamburg, Hamburg, DE — [4]Department of Physics and Astronomy, iNANO, University of Aarhus, Aarhus, DK — [5]Institute of Semiconductor Physics and Solid Solid State Physics, Johannes-Kepler University, Linz, AT

Interfaces between ferromagnetic and non-magnetic Bi2Se3 phases are studied as a material platform to investigate the influence of spin degrees of freedom on 3D topological insulator (TI) properties.

An inverted geometry of n quintuple layers (QLs) Bi2Se3 ontop of Mn-doped Bi2Se3 is achieved by molecular beam epitaxy for n=0 to n=24 QLs and allows to unhamperedly monitor the development of electronic and topological properties by surface sensitive key techniques like angular resolved photoemission spectroscopy. A gap at the Dirac point is observed at small n, which is gradually filled with increasing n. The Dirac point is fully reestablished at about n = 9 QLs. Band bending effects due to the proximity of the interface with the ferromagnetic layers are discussed.

TT 84.8 Fri 11:45 H15

Observation of gapped surface states in the topological regime of the quantum-phase transition in Bi-doped Pb-Sn-Se (111) epitaxial films — •Partha Sarathi Mandal[1], Gunther Springholz[2], Valentyn Volobuev[2], Günther Bauer[2], Evangelos Golias[1], Andrei Varykhalov[1], Jaime Sa'nchez-Barriga[1], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Institut für Halbleiter und Festkörperphysik, Johannes Kepler Universität, Linz, Austria

Topological crystalline insulators are believed to show a straight forward and versatile connection between mirror symmetries and gap opening at the surface Dirac points. Here we systematically studied the trivial-to-topological insulator phase transition [1] of the $Pb_{1-x}Sn_xSe(111)$ surface grown by molecular beam epitaxy and using angle-resolved photoemission spectorscopy (ARPES) under variation of Sn concentration (10 to 28%) and temperature. Differently from the case of the (001) surface [2], we observe two types of Dirac cones centered at $\overline{\Gamma}$ and $\overline{\mathrm{M}}$ in the surface Brillouin zone. By comparing the band structure of samples with fixed Sn concentration and different Bi doping, we demonstrate the existence of gapped surface states within the topological regime of the quantum-phase transition at low temperatures [1].

[1] Y. Ando and L. Fu Annual Review of Condensed Matter Physics Vol. 6: 361-381 (2015). [2] Y. Tanaka, T. Shoman, K. Nakayama, S. Souma, T. Sato, T. Takahashi, M. Novak, Kouji Segawa, and Yoichi Ando PHYSICAL REVIEW B 88, 235126 (2013).

TT 85: Graphene: Electronic Properties & Structure (Joint session of O and TT organized by O)

Time: Friday 10:30–13:00 Location: S051

TT 85.1 Fri 10:30 S051

Graphene tunable transparency to tunneling electrons: A direct tool to measure the local coupling. — •Héctor González Herrero[1], Antonio Javier Martínez Galera[2], Miguel Moreno Ugeda[3], Delia Fernández Torre[4], Pablo Pou[4], Rubén Pérez[4], José María Gómez Rodríguez[1], and Iván Brihuega[1] — [1]Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]CIC nanoGUNE, E-20018 Donostia-San Sebastian, Spain — [4]Dept. Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Graphene grown on metals has proven to be an excellent approach to obtain high quality graphene films. However, special care has to be taken in order to understand the interaction of graphene with the substrate since it can strongly modify its properties.

We have grown one monolayer graphene on Cu (111) by using a new technique. By means of low temperature STM/STS experiments, complemented by density functional theory calculations, we have obtained information about the structural and electronic properties of our graphene samples with atomic precision and high energy resolution. Our work shows that depending on the STM tip apex and the tunnel parameters we can get access to either the graphene layer, the copper surface underneath or even both at the same time. Moreover, this approach can also be applied to investigate the interaction of point defects in the graphene layer with the underlying substrate .

TT 85.2 Fri 10:45 S051

Excitons and the XNLD of higly oriented pyrolytic graphite and graphene - theory and experiment — •Dominik Legut[1], Robert Laskowski[2], Peter M. Oppeneer[3], Christine Jansing[4], Markus Gilbert[4], Andreas Gaupp[4], Hans-Christoph Mertins[4], Andrey Sokolov[5], Suk-Ho Choi[6], Hud Wahab[7], and Heiko Timmers[7] — [1]IT4Innovations Centre, VSB-TU Ostrava, Ostrava, Czech Republic — [2]Institute of High Performance Computing, A*STAR, Singapore — [3]Department of Physics and Astronomy, Uppsala, Sweden — [4]FH Münster, Steinfurt, Germany — [5]HZB, Berlin, Germany — [6]Department of Applied Physics, Kyung Hee University, Korea — [7]University of New South Wales Canberra, Canberra BC, Australia

Reflection spectra of the x-ray natural linear dichroism (XNLD) were calculated on highly oriented pyrolytic graphite (HOPG) and graphene. The π- and σ-excitations stemming from the carbon K-edge are considered. It was computed in the single electron picture within the framework of the standart DFT as the first step. For the better descriptions of the core-hole quasiparticle one can model the 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 HOPG. The spectral shape of the reflectance and XNLD of all three modeles are compared with the experimental data.

TT 85.3 Fri 11:00 S051

Direct measurement of chiral symmetry breaking in strained graphene by STM — Alexander Georgi[1], •Peter Nemes-Incze[1], Ramon Carillo-Bastos[2], Martin Schneider[3], Dinesh Subramaninam[1], Torge Mashoff[4], Daiara Faria[2,5], Silvia Viola Kusminskiy[3], Dawei Zhai[2], Marcus Liebmann[1], Marco Pratzer[1], Ludger Wirtz[6], Nancy Sandler[2], and Markus Morgenstern[1] — [1]RWTH Aachen Univ. and JARA-FIT, Aachen, Germany — [2]Ohio Univ., Athens, Ohio, USA — [3]Freie Univ. Berlin, Berlin, Germany — [4]Johannes Gutenberg-Univ., Mainz, Germany — [5]Univ. Federal Fluminense, Niterói, Brazil — [6]Univ. of Luxembourg, Luxembourg

The breaking of reflection symmetry has important consequences for pseudospin 1/2 particles, such as those used to describe low-energy excitations in graphene. Here we show that forces exerted by the tip of a scanning tunneling microscope induce mechanical strain on sub-nm length scales that acts as a gauge field breaking the chiral symmetry of the system. The parity violation manifests itself as a redistribution of the local density of states between the two sublattices by up to 30%. The effect can be understood as a pseudospin polarization due to a pseudo-Zeeman shift produced by the strain induced pseudo-magnetic field. This interpretation is supported by tight binding simulations and effective Dirac model calculations. The tunable pseudo-magnetic field might be used for the ultra fast separation of electrons of different valleys providing a switchable valley filter as a basic element for valleytronics.

TT 85.4 Fri 11:15 S051

Layer symmetry breaking field and conductivity in graphene twist bilayer — •Nicolas Ray, Sam Shallcross, and Oleg Pankratov — Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany

The rich electronic structure of the graphene twist bilayer includes both a decoupled large angle limit and a strongly coupled small angle limit [1]. We consider the in-plane conductivity via a linearised Boltzmann equation [2] over the full angle range, both with and without a layer-perpendicular electric field. The layer perpendicular electric field is shown to lead to a strong suppression of conductivity at certain "hot spots" in the twist angle and energy phase space.

[1] S. Shallcross et al., Phys. Rev. B 87, 245403, 2013; [2] E. Mariani et al., Phys. Rev. B 86, 165448, 2012.

TT 85.5 Fri 11:30 S051

How partial dislocations may make bilayer graphene both an insulator and a conductor — Heiko Weber[1] and •Sam Shallcross[2] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7 A3, 91058 Erlangen, Germany — [2]Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany

Recently imaged partial dislocations in bilayer graphene [1] have been shown to have a profound impact on transport properties for the case of bilayer graphene on SiC [2]. We demonstrate that the presence of only a few partial dislocations in high quality suspended bilayer graphene can both destroy the intrinsic minimal conductivity of the structurally perfect bilayer, or even enhance it, depending only on the configuration of the partials. The provides a natural explanation for the peculiar behaviour of suspended bilayer graphene, in which seemingly very similar samples are found to be either insulating or conducting in nature.

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer, E. Spiecker, Nature 505, 533 (2014). [2] F. Kisslinger, C. Ott, C. Heide, E. Kampert, B. Butz, E. Spiecker, S. Shallcross, H. B. Weber, Nature Physics 11, 650 (2015).

TT 85.6 Fri 11:45 S051

Electronic structure of partial dislocations in bilayer graphene — Dominik Weckbecker and •Sam Shallcross — Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany

We present electronic structure calculations for the partial dislocations recently imaged in bilayer graphene on SiC [1,2]. We use an effective field method which allows us to treat both a realistic experimental situation of many disordered dislocations in a sample area of a square micrometer as well as model systems in which the dislocations are ordered. We find near the Dirac point a charge pooling on the bilayer graphene segments, as well as a curious energy dependent localization on the partial lines and partial nodes. We consider the presence of an external out-of-plane magnetic field and identify current circulations associated with partial lines.

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer, E. Spiecker, Nature 505, 533 (2014). [2] F. Kisslinger, C. Ott, C. Heide, E. Kampert, B. Butz, E. Spiecker, S. Shallcross, H. B. Weber, Nature Physics 11, 650 (2015).

TT 85.7 Fri 12:00 S051

Deformation in graphene and few layer graphenes: interlayer gauge fields and optical deformations — •Nicolas Ray[1], Fabian Rost[1], Reena Gupta[2], Sangeeta Sharma[2], Oleg Pankratov[1], and Sam Shallcross[1] — [1]Lehrstuhl für theoretische Festkörper-

physik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany — [2]Max-Planck-Institute for Microstructure Physics, Weinberg 2, 06120 Halle, Germany

We present a general theory of deformations in graphene and few layer graphenes. In single layer graphene we consider both acoustic and optical deformations, and show that the latter can generate chiral gap opening fields. For the case of few layer graphenes we derive a general interlayer gauge term that relates the local stacking vector to an off-diagonal non-Abelian field. We show that this general result reduces to well known cases such as the Bernal or twist graphene bilayer, but can also be used to treat more complex situations such as partial dislocations in bilayer graphene.

TT 85.8 Fri 12:15 S051

Substrate nanofacets as a stamp for graphene charge carrier modulations — •Jan Honolka[1], Martin Vondracek[1], Ladislav Fekete[1], Jaromir Kopecek[1], Jan Lancok[1], Dipankar Kalita[2], Johann Coraux[2], and Vincent Bouchiat[2] — [1]Institute of Physics, ASCR, CZ-Prague — [2]Department Nanosciences, CNRS, F-Grenoble

We report on 1D quasiperiodic modulations of graphene electron doping, probed by spatial mapping of the electronic band structure in wave-vector-resolved photoemission microscopy (k-PEEM).

Sampling local topography and diffraction, we show that a nanometer-scale periodic structuration and electronic doping by several 0.1eV can be achieved straightforwardly in graphene, as-grown by CVD on high-index vicinal copper. The pattern consists of a rooftop-like alternance of Cu facets of distinctive symmetries, formed by surface energy minimization at the atomic scale, which drives copper and carbon mass-transfers during high-temperature CVD.

The general concept of this work can be extended towards other chemical vapor deposited 2D systems of current interest such as semiconducting transition metal dichalcogenides, e.g. MoS_2, insulating hexagonal boron nitride (h-BN) monolayers, and respective hybrid structures.

TT 85.9 Fri 12:30 S051

Fermi surface nesting in the graphene twist bilayer — •Maximilian Fleischmann, Dominik Weckbecker, Nicolas Ray, Oleg Pankratov, and Sam Shallcross — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

Two mutually rotated layers of graphene exhibit an electronic structure that depends profoundly on the rotation angle of the two layers [1]. This rich electronic structure invites the possibility of significant band engineering control in the small angle limit [2]. We demonstrate that the small angle limit exhibits a massive Fermi surface nesting in the presence of a perpendicular electric field of strength greater than ~ 100 mV/Å. We describe in detail the unusual band topology in this nested region of the energy field phase space, and discuss some of the many body effects likely to be induced by such strong Fermi surface nesting.

[1] S. Shallcross et al., Phys. Rev. B **87**, 245403, 2013.
[2] D. Weckbecker et al., *submitted*

TT 85.10 Fri 12:45 S051

Force-induced dynamic STM mapping and picking of free-standing graphene membranes — •Bernd Uder, Wolf-Rüdiger Hannes, and Uwe Hartmann — Fachrichtung Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany

Scanning Tunneling Microscopy (STM) of freely suspended membranes only a few atomic layers thick is inherently challenging. Membrane and tip instabilities are easily induced and must be controlled by careful adjustment of scan and regulation parameters. So far only little STM work has been reported on this surface type. We demonstrate seamless imaging of few-layered suspended graphene, from 10μm x 10μm scan width down to 25nm x 25nm. On the scale of 5 - 10nm, we observe corrugations rippled in one dimension. Larger structures are resolved by choosing scan parameters such that vibrational modes are triggered in certain reproducible regions, possibly corresponding to monolayer regions or fragments. Bias voltage ramps are employed for controlled and reversible membrane picking with the observation of flipping processes of the rippled structure.

TT 86: Graphene: Electronic Properties and Structure (Joint session of DS, DY, HL, MA, O and TT organized by O)

Time: Friday 10:30–13:00 Location: S051

TT 86.1 Fri 10:30 S051

Graphene tunable transparency to tunneling electrons: A direct tool to measure the local coupling. — •Héctor González Herrero[1], Antonio Javier Martínez Galera[2], Miguel Moreno Ugeda[3], Delia Fernández Torre[4], Pablo Pou[4], Rubén Pérez[4], José María Gómez Rodríguez[1], and Iván Brihuega[1] — [1]Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]CIC nanoGUNE, E-20018 Donostia-San Sebastian, Spain — [4]Dept. Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Graphene grown on metals has proven to be an excellent approach to obtain high quality graphene films. However, special care has to be taken in order to understand the interaction of graphene with the substrate since it can strongly modify its properties.

We have grown one monolayer graphene on Cu (111) by using a new technique. By means of low temperature STM/STS experiments, complemented by density functional theory calculations, we have obtained information about the structural and electronic properties of our graphene samples with atomic precision and high energy resolution. Our work shows that depending on the STM tip apex and the tunnel parameters we can get access to either the graphene layer, the copper surface underneath or even both at the same time. Moreover, this approach can also be applied to investigate the interaction of point defects in the graphene layer with the underlying substrate .

TT 86.2 Fri 10:45 S051

Excitons and the XNLD of higly oriented pyrolytic graphite and graphene - theory and experiment — •Dominik Legut[1], Robert Laskowski[2], Peter M. Oppeneer[3], Christine Jansing[4], Markus Gilbert[4], Andreas Gaupp[4], Hans-Christoph Mertins[4], Andrey Sokolov[5], Suk-Ho Choi[6], Hud Wahab[7], and Heiko Timmers[7] — [1]IT4Innovations Centre, VSB-TU Ostrava, Ostrava, Czech Republic — [2]Institute of High Performance Computing, A*STAR, Singapore — [3]Department of Physics and Astronomy, Uppsala, Sweden — [4]FH Münster, Steinfurt, Germany — [5]HZB, Berlin, Germany — [6]Department of Applied Physics, Kyung Hee University, Korea — [7]University of New South Wales Canberra, Canberra BC, Australia

Reflection spectra of the x-ray natural linear dichroism (XNLD) were calculated on highly oriented pyrolytic graphite (HOPG) and graphene. The π- and σ-excitations stemming from the carbon K-edge are considered. It was computed in the single electron picture within the framework of the standart DFT as the first step. For the better descriptions of the core-hole quasiparticle one can model the 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 HOPG. The spectral shape of the reflectance and XNLD of all three modeles are compared with the experimental data.

TT 86.3 Fri 11:00 S051

Direct measurement of chiral symmetry breaking in strained graphene by STM — Alexander Georgi[1], •Peter Nemes-Incze[1], Ramon Carillo-Bastos[2], Martin Schneider[3], Dinesh Subramaninam[1], Torge Mashoff[4], Daiara Faria[2,5], Silvia Viola Kusminskiy[3], Dawei Zhai[2], Marcus Liebmann[1], Marco Pratzer[1], Ludger Wirtz[6], Nancy Sandler[2], and Markus Morgenstern[1] — [1]RWTH Aachen Univ. and JARA-FIT, Aachen, Germany — [2]Ohio Univ., Athens, Ohio, USA — [3]Freie Univ. Berlin, Berlin, Germany — [4]Johannes Gutenberg-Univ., Mainz, Germany —

[5]Univ. Federal Fluminense, Niterói, Brazil — [6]Univ. of Luxembourg, Luxembourg

The breaking of reflection symmetry has important consequences for pseudospin 1/2 particles, such as those used to describe low-energy excitations in graphene. Here we show that forces exerted by the tip of a scanning tunneling microscope induce mechanical strain on sub-nm length scales that acts as a gauge field breaking the chiral symmetry of the system. The parity violation manifests itself as a redistribution of the local density of states between the two sublattices by up to 30%. The effect can be understood as a pseudospin polarization due to a pseudo-Zeeman shift produced by the strain induced pseudo-magnetic field. This interpretation is supported by tight binding simulations and effective Dirac model calculations. The tunable pseudo-magnetic field might be used for the ultra fast separation of electrons of different valleys providing a switchable valley filter as a basic element for valleytronics.

TT 86.4 Fri 11:15 S051

Layer symmetry breaking field and conductivity in graphene twist bilayer — •Nicolas Ray, Sam Shallcross, and Oleg Pankratov — Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany

The rich electronic structure of the graphene twist bilayer includes both a decoupled large angle limit and a strongly coupled small angle limit [1]. We consider the in-plane conductivity via a linearised Boltzmann equation [2] over the full angle range, both with and without a layer-perpendicular electric field. The layer perpendicular electric field is shown to lead to a strong suppression of conductivity at certain "hot spots" in the twist angle and energy phase space.

[1] S. Shallcross et al., Phys. Rev. B 87, 245403, 2013; [2] E. Mariani et al., Phys. Rev. B 86, 165448, 2012.

TT 86.5 Fri 11:30 S051

How partial dislocations may make bilayer graphene both an insulator and a conductor — Heiko Weber[1] and •Sam Shallcross[2] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7 A3, 91058 Erlangen, Germany — [2]Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany

Recently imaged partial dislocations in bilayer graphene [1] have been shown to have a profound impact on transport properties for the case of bilayer graphene on SiC [2]. We demonstrate that the presence of only a few partial dislocations in high quality suspended bilayer graphene can both destroy the intrinsic minimal conductivity of the structurally perfect bilayer, or even enhance it, depending only on the configuration of the partials. The provides a natural explanation for the peculiar behaviour of suspended bilayer graphene, in which seemingly very similar samples are found to be either insulating or conducting in nature.

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer, E. Spiecker, Nature 505, 533 (2014). [2] F. Kisslinger, C. Ott, C. Heide, E. Kampert, B. Butz, E. Spiecker, S. Shallcross, H. B. Weber, Nature Physics 11, 650 (2015).

TT 86.6 Fri 11:45 S051

Electronic structure of partial dislocations in bilayer graphene — Dominik Weckbecker and •Sam Shallcross — Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany

We present electronic structure calculations for the partial dislocations recently imaged in bilayer graphene on SiC [1,2]. We use an effective field method which allows us to treat both a realistic experimental situation of many disordered dislocations in a sample area of a square micrometer as well as model systems in which the dislocations are ordered. We find near the Dirac point a charge pooling on the bilayer graphene segments, as well as a curious energy dependent localization on the partial lines and partial nodes. We consider the presence of an external out-of-plane magnetic field and identify current circulations associated with partial lines.

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer, E. Spiecker, Nature 505, 533 (2014). [2] F. Kisslinger, C. Ott, C. Heide, E. Kampert, B. Butz, E. Spiecker, S. Shallcross, H. B. Weber, Nature Physics 11, 650 (2015).

TT 86.7 Fri 12:00 S051

Deformation in graphene and few layer graphenes: interlayer gauge fields and optical deformations — •Nicolas Ray[1], Fabian Rost[1], Reena Gupta[2], Sangeeta Sharma[2], Oleg Pankratov[1], and Sam Shallcross[1] — [1]Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany — [2]Max-Planck-Institute for Microstructure Physics, Weinberg 2, 06120 Halle, Germany

We present a general theory of deformations in graphene and few layer graphenes. In single layer graphene we consider both acoustic and optical deformations, and show that the latter can generate chiral gap opening fields. For the case of few layer graphenes we derive a general interlayer gauge term that relates the local stacking vector to an off-diagonal non-Abelian field. We show that this general result reduces to well known cases such as the Bernal or twist graphene bilayer, but can also be used to treat more complex situations such as partial dislocations in bilayer graphene.

TT 86.8 Fri 12:15 S051

Substrate nanofacets as a stamp for graphene charge carrier modulations — •Jan Honolka[1], Martin Vondracek[1], Ladislav Fekete[1], Jaromir Kopecek[1], Jan Lancok[1], Dipankar Kalita[2], Johann Coraux[2], and Vincent Bouchiat[2] — [1]Institute of Physics, ASCR, CZ-Prague — [2]Department Nanosciences, CNRS, F-Grenoble

We report on 1D quasiperiodic modulations of graphene electron doping, probed by spatial mapping of the electronic band structure in wave-vector-resolved photoemission microscopy (k-PEEM).

Sampling local topography and diffraction, we show that a nanometer-scale periodic structuration and electronic doping by several 0.1eV can be achieved straightforwardly in graphene, as-grown by CVD on high-index vicinal copper. The pattern consists of a rooftop-like alternance of Cu facets of distinctive symmetries, formed by surface energy minimization at the atomic scale, which drives copper and carbon mass-transfers during high-temperature CVD.

The general concept of this work can be extended towards other chemical vapor deposited 2D systems of current interest such as semiconducting transition metal dichalcogenides, e.g. MoS_2, insulating hexagonal boron nitride (h-BN) monolayers, and respective hybrid structures.

TT 86.9 Fri 12:30 S051

Fermi surface nesting in the graphene twist bilayer — •Maximilian Fleischmann, Dominik Weckbecker, Nicolas Ray, Oleg Pankratov, and Sam Shallcross — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

Two mutually rotated layers of graphene exhibit an electronic structure that depends profoundly on the rotation angle of the two layers [1]. This rich electronic structure invites the possibility of significant band engineering control in the small angle limit [2]. We demonstrate that the small angle limit exhibits a massive Fermi surface nesting in the presence of a perpendicular electric field of strength greater than ~ 100 mV/Å. We describe in detail the unusual band topology in this nested region of the energy field phase space, and discuss some of the many body effects likely to be induced by such strong Fermi surface nesting.

[1] S. Shallcross et al., Phys. Rev. B **87**, 245403, 2013.
[2] D. Weckbecker et al., *submitted*

TT 86.10 Fri 12:45 S051

Force-induced dynamic STM mapping and picking of free-standing graphene membranes — •Bernd Uder, Wolf-Rüdiger Hannes, and Uwe Hartmann — Fachrichtung Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany

Scanning Tunneling Microscopy (STM) of freely suspended membranes only a few atomic layers thick is inherently challenging. Membrane and tip instabilities are easily induced and must be controlled by careful adjustment of scan and regulation parameters. So far only little STM work has been reported on this surface type. We demonstrate seamless imaging of few-layered suspended graphene, from 10μm x 10μm scan width down to 25nm x 25nm. On the scale of 5 - 10nm, we observe corrugations rippled in one dimension. Larger structures are resolved by choosing scan parameters such that vibrational modes are triggered in certain reproducible regions, possibly corresponding to monolayer regions or fragments. Bias voltage ramps are employed for controlled and reversible membrane picking with the observation of flipping processes of the rippled structure.